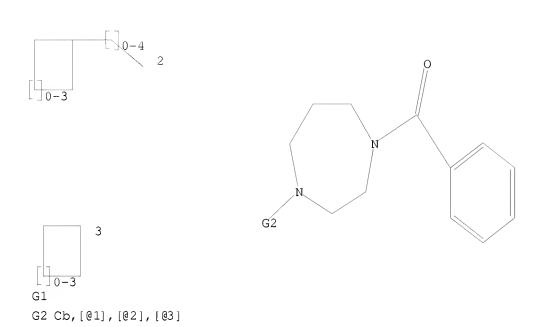
```
=> d his
     (FILE 'HOME' ENTERED AT 22:06:16 ON 21 OCT 2009)
    FILE 'REGISTRY' ENTERED AT 22:06:23 ON 21 OCT 2009
    FILE 'CAPLUS' ENTERED AT 22:06:26 ON 21 OCT 2009
L1
             1 S US 20080045505/PN
               SELECT RN L1 1-
    FILE 'REGISTRY' ENTERED AT 22:06:43 ON 21 OCT 2009
           138 S E1-138
L2
            69 S L2 AND 7/SZ
L3
L4
            62 S L3 AND NRS>2
    FILE 'CAPLUS' ENTERED AT 22:10:02 ON 21 OCT 2009
L5
           1 S L4
    FILE 'REGISTRY' ENTERED AT 22:15:19 ON 21 OCT 2009
L6
               STRUCTURE UPLOADED
            50 S L6
L7
          3697 S L6 SSS FUL
L8
L9
           176 S L8 AND CYCLOPROP?
           147 S L8 AND CYCLOBUT?
L10
L11
            24 S L8 AND CYCLOPEN?
L12
           232 S L8 AND CYCLOHEX?
            1 S L8 AND CYCLOHEP?
L13
           572 S L9 OR L10 OR L11 OR L12 OR L13
L14
    FILE 'CAPLUS' ENTERED AT 22:20:01 ON 21 OCT 2009
L15
           20 S L14
L16
            16 S L15 NOT (2009/SO OR 2008/SO OR 2007/SO OR 2006/SO OR 2005/SO)
=> d 16
L6 HAS NO ANSWERS
```

L6

STR

Ak 1



Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr total

L16 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:617753 CAPLUS

DOCUMENT NUMBER: 150:563845

TITLE: Preparation of pyridazinone derivatives as inhibitors

of poly(adp-ribose)polymerase (parp)

INVENTOR(S):

Branca, Danila; Dessole, Gabriella; Ferrigno,
Federica; Jones, Philip; Kinzel, Olaf; Lillini,
Samuele; Muraglia, Ester; Pescatore, Giovanna;

Schultz-Fademrecht, Carsten

PATENT ASSIGNEE(S): Istituto di Ricerche di Biologia Molecolare P.

Angeletti S.p.A., Italy

SOURCE: PCT Int. Appl., 141pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PAT | PATENT NO. | | | | KIND DATE | | APPLICATION NO. | | | | | | DATE | | | | |
|----------|-----------------------|-----|-----|-------------|-----------|-------------------|-----------------|-----|---------------|------|------|----------|------|-----|------------|------|-----|
| WO | WO 2009063244 | | | A1 20090522 | | WO 2008-GB51063 | | | | | | 20081114 | | | | | |
| | W: | ΑE, | AG, | AL, | AM, | AO, | AT, | ΑU, | AZ, | BA, | BB, | BG, | BH, | BR, | BW, | BY, | BZ, |
| | | CA, | CH, | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DO, | DZ, | EC, | EE, | EG, | ES, |
| | | FI, | GB, | GD, | GE, | GH, | GM, | GT, | HN, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, |
| | | KG, | KM, | KN, | KP, | KR, | KΖ, | LA, | LC, | LK, | LR, | LS, | LT, | LU, | LY, | MA, | MD, |
| | | ME, | MG, | MK, | MN, | MW, | MX, | MY, | MΖ, | NA, | NG, | NΙ, | NO, | NZ, | OM, | PG, | PH, |
| | | PL, | PT, | RO, | RS, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SM, | ST, | SV, | SY, | TJ, |
| | | TM, | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UΖ, | VC, | VN, | ZA, | ZM, | ZW | | |
| | RW: | AT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HR, | HU, |
| | | ΙE, | IS, | ΙΤ, | LT, | LU, | LV, | MC, | MΤ, | NL, | NO, | PL, | PT, | RO, | SE, | SI, | SK, |
| | | TR, | BF, | ВJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | NE, | SN, | TD, |
| | | ΤG, | BW, | GH, | GM, | ΚE, | LS, | MW, | MΖ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, |
| | | AM, | AZ, | BY, | KG, | ΚZ, | MD, | RU, | ТJ, | TM | | | | | | | |
| PRIORITY | RIORITY APPLN. INFO.: | | | . : | | | | | GB 2007-22401 | | | | | 1 | A 20071115 | | |
| | | | | | | | | | (| GB 2 | -800 | 1670 | 7 | i | A 2 | 0080 | 912 |
| OTHER SO | THER SOURCE(S): | | | | MAR | MARPAT 150:563845 | | | | | | | | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compound I [m, n = independently 0-1; X = (CH2)d; d = 1-2; R = [(CR3R4)eR5]f; e, f, q = independently 0-4; A = 6-15 membered monocyclyl, fused, bridged or spiro saturated heterocyclyl containing 2 N's and 0-1 O, substituted by one oxo group; R1 = independently at each occurrence alkyl, haloalkyl, halo, CN; R2 = independently at each occurrence OH, halo, R1, OH, alkoxy, haloalkoxy, NH2 and derivs.; R3, R4 = independently at each occurrence H, halo, alkyl, haloalkyl; R5 = independently at each occurrence R1, alkenyl, alkoxycarbonyl, (un)substituted cycloalkyl, aryl, azetidinyl, etc.], and their pharmaceutically acceptable salts, stereoisomers and tautomers were prepared and disclosed as inhibitors of poly(adp-ribose)polymerase (parp). Thus, reacting 5-[(4,5-dimethyl-6-oxo-1,6-dihydropyridazin-3-yl)methyl]-2-fluorobenzoicacid(preparation given) with 1-cyclohexyl-3,3-dimethylpiperazin-2-one (preparation given) gave II•TFA.

GI

Selected I showed an IC50 value of less than 5 μM in a PARP-1 SPA assay. I were tested in an antiproliferative assay in matched pair BRCA1wt and BRCA1-(shRNA) HeLa cells. The majority of compds. I showed a CC50 less than 5 μM in BRCA1 deficient cells and a greater than 50 fold selectivity over the BRCA proficient cells. I should prove useful for the treatment of cancer, inflammatory diseases, reperfusion injuries, ischemic conditions, stroke, renal failure, cardiovascular diseases, vascular diseases other than cardiovascular diseases, diabetes mellitus, neurodegenerative diseases, retroviral infections, retinal damage, skin senescence and UV-induced skin damage, and as chemo- or radiosensitizers for cancer treatment.

IT 1154869-36-9P 1154870-76-4P,

1- Cyclopropyl-4-[5-[(4,5-dimethyl-6-oxo-1,6-dihydropyridazin-3-yl)methyl]-2-fluorobenzoyl]-1,4-diazepan-2-one

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyridazinone derivs. as inhibitors of poly(adp-ribose)polymerase)

RN 1154869-36-9 CAPLUS

CN 2H-1,4-Diazepin-2-one, 1-cyclohexyl-4-[5-[(1,6-dihydro-4,5-dimethyl-6-oxo-3-pyridazinyl)methyl]-2-fluorobenzoyl]hexahydro-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1154869-35-8 CMF C25 H31 F N4 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 1154870-76-4 CAPLUS

CN 2H-1,4-Diazepin-2-one, 1-cyclopropyl-4-[5-[(1,6-dihydro-4,5-dimethyl-6-oxo-3-pyridazinyl)methyl]-2-fluorobenzoyl]hexahydro- (CA INDEX NAME)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:237998 CAPLUS

DOCUMENT NUMBER: 150:283083

TITLE: Preparation of piperazine derivatives as LXR

modulators

INVENTOR(S): Ho, Koc-Kan; Roughton, Andrew Laird; Neagu, Irina;

Chan, Jui-Hsiang; Ansari, Nasrin; Morris, Michelle Lee; Rong, Yajing; Ohlmeyer, Michael; Cooke, Andrew

John; Edwards, Andrew Stanley; Bennett, David Jonathan

PATENT ASSIGNEE(S): N.V. Organon, Neth. SOURCE: PCT Int. Appl., 105pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA: | PATENT NO. | | | | | KIND DATE | | | APPLICATION NO. | | | | | | DATE | | | |
|------------------------|---------------|-----|-----|-----|----------------|-----------|-----|-----------------|-----------------|-----|------------|-----|----------|-----|------|-----|-----|--|
| WO | WO 2009024550 | | | A1 | A1 20090226 | | | WO 2008-EP60788 | | | | | 20080818 | | | | | |
| | W: | ΑE, | AG, | AL, | AM, | AO, | AT, | AU, | ΑZ, | BA, | BB, | BG, | BH, | BR, | BW, | BY, | BZ, | |
| | | CA, | CH, | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DO, | DZ, | EC, | EE, | EG, | ES, | |
| | | FI, | GB, | GD, | GE, | GH, | GM, | GT, | HN, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KΕ, | |
| | | KG, | KM, | KN, | KP, | KR, | KΖ, | LA, | LC, | LK, | LR, | LS, | LT, | LU, | LY, | MA, | MD, | |
| | | ME, | MG, | MK, | MN, | MW, | MX, | MY, | MZ, | NA, | NG, | ΝI, | NO, | NZ, | OM, | PG, | PH, | |
| | | PL, | PT, | RO, | RS, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SM, | ST, | SV, | SY, | ТJ, | |
| | | TM, | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UΖ, | VC, | VN, | ZA, | ZM, | ZW | | | |
| | RW: | ΑT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HR, | HU, | |
| | | ΙE, | IS, | ΙΤ, | LT, | LU, | LV, | MC, | MT, | NL, | NO, | PL, | PT, | RO, | SE, | SI, | SK, | |
| | | TR, | BF, | ВJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | ΝE, | SN, | TD, | |
| | | TG, | BW, | GH, | GM, | ΚE, | LS, | MW, | MΖ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | |
| | | ΑM, | ΑZ, | BY, | KG, | KΖ, | MD, | RU, | ΤJ, | TM | | | | | | | | |
| PRIORITY APPLN. INFO.: | | | | | EP 2007-114602 | | | | | 1 | A 20070820 | | | | | | | |

OTHER SOURCE(S): MARPAT 150:283083

GΙ

AΒ The invention relates to piperazine derivs. having the general formula I to pharmaceutical compns. comprising the same, and to the use of these compds. for the manufacture of a medicament for treating or preventing atherosclerosis and related disorders associated with cholesterol and bile acids transport and metabolism Compds. of formula I [n = 1-2; A = 6-membered]aromatic ring; X = NR8, O or bond; R1 = H, (un)substituted alkyl, alkyloxy, alkyloxycarbonyl, cycloalkyl, etc.; R2 = alkyl, alkyloxy, CF3 or halogen; R3 = (un)substituted alkyl; R4 = H or alkyl; R5 = alkyl, alkyloxy or halo; R6 = H, (un)substituted alkyl, cycloalkyl, cycloalkyl-alkyl, or a 5- or 6-membered (hetero)aryl; R7 = H or alkyl; R8 = H or alkyl; NR1R8 = 4- to 8-membered (hetero)cyclyl], and their pharmaceutically acceptable salts, are prepared and disclosed. Thus, e.g., acylation of N-tert-Butyl-3-[(piperazin-1-yl)methyl]benzamide dihydrochloride (preparation given) with 4-nitrobenzoyl chloride followed by reduction to give intermediate $3-[[4-(4-aminobenzoyl)piperazin-1-yl]methyl]-N-tert-butylbenzamide\ which$ was treated with 4-nitrophenyl chloroformate and (cyclopropylmethyl)amine gave trifluoroacetate salt of II. Active compds. of the invention showed pKi values > 5.5 with the binding to LXR α using purified ligand binding domain (LBD) in radioligand competition binding scintillation proximity assay.

IT 1124214-57-8P, N-tert-Butyl-3-[[4-[4-(3-cyclobutylureido)benzoyl]-1,4-diazepan-1-yl]methyl]benzamide 2,2,2-trifluoroacetate

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperazine derivs. as LXR modulators)

RN 1124214-57-8 CAPLUS

CN Benzamide, 3-[[4-[4-[[(cyclobutylamino)carbonyl]amino]benzoyl]hexahydro-1H-1,4-diazepin-1-yl]methyl]-N-(1,1-dimethylethyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

10/576,492

CM 1

CRN 1124214-56-7 CMF C29 H39 N5 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT:

6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:1310203 CAPLUS

DOCUMENT NUMBER: 149:513842

TITLE: Preparation of fused pyridazine derivatives as

inhibitors of poly(ADP-ribose)polymerase

INVENTOR(S): Gandhi, Virajkumar B.; Giranda, Vincent L.; Gong,

Jianchun; Penning, Thomas D.; Zhu, Gui-Dong

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: U.S. Pat. Appl. Publ., 162pp., Cont.-in-part of U.S.

Ser. No. 964,822.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-------------------|------------|
| | | | | |
| US 20080269234 | A1 | 20081030 | US 2008-138168 | 20080612 |
| AU 2007340020 | A1 | 20080710 | AU 2007-340020 | 20071220 |
| CA 2672868 | A1 | 20080710 | CA 2007-2672868 | 20071220 |
| KR 2009094116 | A | 20090903 | KR 2009-713523 | 20071220 |
| US 20080161280 | A1 | 20080703 | US 2007-964822 | 20071227 |
| PRIORITY APPLN. INFO.: | | | US 2006-882317P P | 20061228 |
| | | | US 2007-964822 A | 2 20071227 |
| | | | WO 2007-US88319 W | 20071220 |

OTHER SOURCE(S): MARPAT 149:513842

GΙ

AB The title compds. [I; wherein A1 = each (un)substituted R1 or R2; R1 = cycloalkane or cycloalkene, each of which is (un)fused with R1A; R2 = heterocycloalkane or heterocycloalkene, each of which is (un)fused with R2A; R1A, R2A = benzene, heteroarene, cycloalkane, cycloalkene, heterocycloalkane or heterocycloalkene; A2 = OR4, NHR4, N(R4)2, SR4, S(0)R4, S02R4, or R5; R4 = C1-3 alkyl substituted with R5; R5 = C1-5 alkyl substituted with R10, and further unsubstituted or substituted with one or two or three of independently selected OR10, NHR10, N(R10)2, SR10, S(0)R10, S02R10 or CF3; R10 = each (un)substituted R10A, R10B or R10C,

each of which must be attached at a carbon atom; R10A = each (un)fused Ph; R10B = each (un)fused 2- or 3-pyridyl, 4- or 5-pyrimidinyl, 2- or 3-thienyl, 2-, 4-, 5-thiazolyl or 2-, 4-, 5-oxazolyl; R10C = each(un) fused cycloalkyl, cycloalkenyl, heterocycloalkyl or heterocycloalkenyl] or pharmaceutically acceptable salts thereof were prepared These compds. are inhibitors of poly(ADP-ribose)polymerase (PARP) and are useful for treating cancer optionally in combination with radiotherapy or a chemotherapeutic agent selected from temozolomide, dacarbazine, cyclophosphamide, carmustine, melphalan, lomustine, carboplatin, cisplatin, 5-fluorouracil, leucovorin, gemcitabine, methotrexate, bleomycin, irinotecan, camptothecin, or topotecan. Thus, 100 mg 2-fluoro-5-[(4-oxo-3,4,5,6,7,8-hexahydrophthalazin-1yl)methyl]benzoic acid was stirred with 126 mg 2-(1H-7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate methanaminium (HATU) and 92 μL triethylamine and stirred for 20 min at room temperature, treated with 78 mg (piperazin-1-yl)pyrimidine dihydrochloride, and then stirred at room temperature

for 16 h to give 4-[4-fluoro-3-[(4-pyrimidin-2-ylpiperazin-1-yl)carbonyl]benzyl]-5,6,7,8-tetrahydrophthalazin-1(2H)-one (II). II inhibited PARP-1 with Ki of 0.7 nM and showed the inhibition of the formation of poly ADP-ribose in C41 cell with EC50 of 0.7 nM.

IT 1073657-08-5P 1073657-09-6P 1073657-11-0P 1073657-12-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of fused pyridazine derivs. as inhibitors of poly(ADP-ribose)polymerase for treating cancer)

RN 1073657-08-5 CAPLUS

CN 1(2H)-Phthalazinone, 4-[[3-[[4-(cyclopropylcarbonyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-4-fluorophenyl]methyl]-5,6,7,8-tetrahydro- (CA INDEX NAME)

RN 1073657-09-6 CAPLUS

CN 1(2H)-Phthalazinone, 4-[[3-[[4-(cyclopropylcarbonyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-4-fluorophenyl]methyl]-5,6,7,8-tetrahydro-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1073657-08-5 CMF C25 H29 F N4 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 1073657-11-0 CAPLUS
CN 1(2H)-Phthalazinone, 4-[[4-fluoro-3-[[hexahydro-4-[(1-methylcyclopropyl)carbonyl]-1H-1,4-diazepin-1-yl]carbonyl]phenyl]methyl]-5,6,7,8-tetrahydro- (CA INDEX NAME)

RN 1073657-12-1 CAPLUS

CN 1(2H)-Phthalazinone, 4-[[4-fluoro-3-[[hexahydro-4-[(1-methylcyclopropyl)carbonyl]-1H-1,4-diazepin-1-yl]carbonyl]phenyl]methyl]-5,6,7,8-tetrahydro-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1073657-11-0 CMF C26 H31 F N4 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

L16 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:639210 CAPLUS

DOCUMENT NUMBER: 149:9893

TITLE: Preparation of substituted phenyl propyl amines as

histamine H3 receptor and serotonin transporter

modulators

INVENTOR(S): Keith, John M.; Miller, Jennifer M. B.; Stocking,

Emily M.

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 92pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| | PATENT NO. | | | | | KIND | | DATE | | APPLICATION NO. | | | | | | DATE | | |
|-------|------------------|------|------|------|------|----------|------|-----------------|------|-----------------|------|------|----------|------------|-----|------|------|-----|
| | WO 2008064036 | | | A1 | _ | 20080529 | | WO 2007-US84657 | | | | | 20071114 | | | | | |
| | | W: | ΑE, | AG, | AL, | AM, | ΑT, | ΑU, | ΑZ, | BA, | BB, | BG, | BH, | BR, | BW, | BY, | BZ, | CA, |
| | | | CH, | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DO, | DZ, | EC, | EE, | EG, | ES, | FI, |
| | | | GB, | GD, | GE, | GH, | GM, | GT, | HN, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, |
| | | | KM, | KN, | KP, | KR, | ΚZ, | LA, | LC, | LK, | LR, | LS, | LT, | LU, | LY, | MA, | MD, | ME, |
| | | | MG, | MK, | MN, | MW, | MX, | MY, | MZ, | NA, | NG, | NI, | NO, | NΖ, | OM, | PG, | PH, | PL, |
| | | | PT, | RO, | RS, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SM, | SV, | SY, | ТJ, | TM, | TN, |
| | | | TR, | TT, | TZ, | UA, | UG, | US, | UΖ, | VC, | VN, | ZA, | ZM, | zw | | | | |
| | | RW: | ΑT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HU, | ΙE, |
| | | | IS, | IT, | LT, | LU, | LV, | MC, | MT, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR, | BF, |
| | | | ВJ, | CF, | CG, | CI, | CM, | GΑ, | GN, | GQ, | GW, | ML, | MR, | ΝE, | SN, | TD, | TG, | BW, |
| | | | GH, | GM, | ΚE, | LS, | MW, | ΜZ, | NA, | SD, | SL, | SZ, | ΤZ, | UG, | ZM, | ZW, | AM, | ΑZ, |
| | | | BY, | KG, | KΖ, | MD, | RU, | ТJ, | TM | | | | | | | | | |
| | US | 2008 | 0139 | 564 | | A1 | | 2008 | 0612 | | US 2 | 007- | 9398 | 81 | | 2 | 0071 | 114 |
| PRIOR | RITY | APP: | LN. | INFO | .: | | | | | US 2006-866112P | | | | P 20061116 | | | | |
| OTHER | OTHER SOURCE(S): | | | | MAR: | PAT | 149: | 9893 | | | | | | | | | | |
| GI | | | | | | | | | | | | | | | | | | |

The title compds. I [one of X and Y = O, S, NH or CH2, and the other is a AB bond; Z = CH or N, with the proviso that Z = N only when Y = O; one of R1 and R2 = Q and the other = H; Q = OCHRa(CH2)2NRbRc, C.tplbond.C(CH2)2NRbRc, (CH2)4NRbRc, CH2NRbRc or C(O)NRbRc (wherein Ra = H or is taken together with Rb to form ethylene; Rb and Rc = H or alkyl, or NRbRc = (un)substituted heterocycloalkyl); R4 = halo, alkyl, CHF2, etc.; n = 0-3; R5 = H or alkyl; R6 = alkyl; or NR5R6 = heterocycloalkyl; and their pharmaceutically acceptable salts] which are histamine H3 receptor and/or serotonin transporter modulators useful in the treatment of histamine H3 receptor- and/or serotonin-mediated diseases, were prepared E.g., a multi-step synthesis of II. maleate, starting from 1-(4-hydroxyphenyl)ethanone and 1-bromo-3-chloropropane, was given. Exemplified compds. I were tested in various biol. tests (data given for representative compds. I). Pharmaceutical composition comprising the compound Ι

was disclosed.

IT 1029649-31-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted phenylpropylamines as histamine H3 receptor and serotonin transporter modulators useful in treatment of histamine H3 receptor— and serotonin—mediated diseases)

RN 1029649-31-7 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-[3-(dimethylamino)-1-[4-(trifluoromethyl)phenoxy]propyl]phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} O & CH_2-CH_2-NMe_2 \\ \hline CH-O & CF_3 \end{array}$$

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:12128 CAPLUS

DOCUMENT NUMBER: 148:100642

TITLE: Preparation of substituted aminomethyl benzamides as

histamine H3 receptor and serotonin transporter

modulators

INVENTOR(S): Allison, Brett; Carruthers, Nicholas I.; Curtis,

Michael P.; Keith, John M.; Letavic, Michael A.;

Stocking, Emily M.

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 73pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA' | PATENT NO. | | | | KIND DATE | | | APPLICATION NO. | | | | | | DATE | | | |
|----------|-----------------|------|------|-----|-------------|--------------|---------------|-----------------|-----------------|------|-------|------|---------|------|----------|------|-----|
| WO | 2008 | 0028 | 18 | | A1 | - | 2008 | 0103 | | WO 2 | 2007- | us71 | 739 | | 2 | 0070 | 621 |
| | W: | ΑE, | AG, | AL, | AM, | AT, | AU, | AZ, | BA, | BB, | BG, | BH, | BR, | BW, | BY, | BZ, | CA, |
| | | CH, | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DO, | DZ, | EC, | EE, | EG, | ES, | FI, |
| | | GB, | GD, | GE, | GH, | GM, | GT, | HN, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, |
| | | KM, | KN, | KP, | KR, | KΖ, | LA, | LC, | LK, | LR, | LS, | LT, | LU, | LY, | MA, | MD, | ME, |
| | | MG, | MK, | MN, | MW, | MX, | MY, | MZ, | NA, | NG, | NI, | NO, | NZ, | OM, | PG, | PH, | PL, |
| | | PT, | RO, | RS, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SM, | SV, | SY, | ΤJ, | TM, | TN, |
| | | TR, | TT, | TZ, | UA, | UG, | US, | UZ, | VC, | VN, | ZA, | ZM, | ZW | | | | |
| | RW: | AT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HU, | IE, |
| | | IS, | IT, | LT, | LU, | LV, | MC, | MT, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR, | BF, |
| | | ВJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | ΝE, | SN, | TD, | TG, | BW, |
| | | GH, | GM, | ΚE, | LS, | MW, | MZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | AZ, |
| | | BY, | KG, | KΖ, | MD, | RU, | ТJ, | TM | | | | | | | | | |
| AU | 2007 | 2652 | 40 | | A1 | | 2008 | 0103 | | AU 2 | 2007- | 2652 | 40 | | 2 | 0070 | 621 |
| CA | 2656 | 083 | | | A1 20080103 | | | | CA 2007-2656083 | | | | | | 20070621 | | |
| US | 2008 | 0045 | 508 | | A1 20080221 | | | | US 2007-766153 | | | | | | 2 | 0070 | 621 |
| EP | 2046 | 747 | | | A1 | | 2009 | 0415 | | EP 2 | 2007- | 7988 | 63 | | 2 | 0070 | 621 |
| | R: | AT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HU, | IE, |
| | | IS, | IT, | LI, | LT, | LU, | LV, | MC, | ΜT, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR, |
| | | AL, | BA, | HR, | MK, | RS | | | | | | | | | | | |
| CN | 1015 | 1179 | 0 | | A | | 2009 | 0819 | | CN 2 | 2007- | 8003 | 2397 | | 2 | 0090 | 302 |
| PRIORIT | Y APP | LN. | INFO | .: | | | | | | US 2 | 2006- | 8061 | 67P |] | P 2 | 0060 | 629 |
| | | | | | | | | | | WO 2 | 2007- | US71 | 739 | Ţ | W 2 | 0070 | 621 |
| OTHER SO | THER SOURCE(S): | | | | MAR | PAT | AT 148:100642 | | | | | | | | | | |

OTHER SOURCE(S): MARPAT 148:100642

GΙ

Cyc
$$R^{11}$$
 Y
 R^{6}
 N
 R^{7}
 R^{5}
 I
 R^{2}
 N
 O
 II

AB The title compds. I [one of R11 and R12 = II and the other = H; Y = O, OCH2, S, SO, SO2; R2 = H, (un)substituted alkyl, cycloalkyl; R5 = H, alkyl; R6, R7 = H, alkyl, cycloalkyl, etc.; or NR6R7 = (un)substituted saturated monocyclic heterocycloalkyl; Cyc = (un)substituted Ph or monocyclic carbon-linked heteroaryl] that are histamine H3 receptor and/or serotonin transporter modulators useful in the treatment of histamine H3 receptorand/or serotonin-mediated diseases, were prepared E.g., a multi-step synthesis of III, starting from 5-bromo-2-fluorobenzaldehyde and 3,4-dichlorophenol, was given. Exemplified compds. I were tested in H3 receptor binding assay and rat brain SERT assay. For example, III showed Ki of 1.8 nM in human H3 assay and Ki of 9.1 nM in rat SERT assay. Pharmaceutical compns. comprising compound I alone or in combination with other therapeutic agent are disclosed.

III

| ΙT | 1000391-96-7P | 1000391-97-8P | 1000391-99-0P |
|----|------------------------|---------------|---------------|
| | 1000392-00-6P | 1000392-01-7P | 1000392-02-8P |
| | 1000392-03-9P | 1000392-04-0P | 1000392-05-1P |
| | 1000392-07-3P | 1000392-08-4P | 1000392-09-5P |
| | 1000392-11-9P | 1000392-12-0P | 1000392-13-1P |
| | 1000392-14 - 2P | 1000392-15-3P | 1000392-16-4P |
| | 1000392-17-5P | 1000392-18-6P | 1000392-19-7P |
| | 1000392-21-1P | 1000392-22-2P | 1000392-23-3P |
| | 1000392-24-4P | 1000392-25-5P | 1000392-26-6P |
| | 1000392-27-7P | 1000392-28-8P | 1000392-29-9P |
| | 1000392-30-2P | 1000392-31-3P | 1000392-32-4P |
| | 1000392-33-5P | 1000392-34-6P | 1000392-35-7P |
| | 1000392-36-8P | 1000392-37-9P | 1000392-42-6P |
| | 1000392-43-7P | 1000392-46-0P | 1000392-47-1P |
| | 1000392-49-3P | | |
| | | | |

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10/576,492

(preparation of substituted aminomethyl benzamides as histamine H3 receptor and serotonin transporter modulators for treating histamine H3 receptor— and serotonin—mediated diseases)

RN 1000391-96-7 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(3,4-dichlorophenoxy)-3-[(methylamino)methyl]phenyl]- (CA INDEX NAME)

RN 1000391-97-8 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[3-[(methylamino)methyl]-4-[4-(trifluoromethyl)phenoxy]phenyl]- (CA INDEX NAME)

RN 1000391-99-0 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[3-[(methylamino)methyl]-4-(3-pyridinyloxy)phenyl]- (CA INDEX NAME)

RN 1000392-00-6 CAPLUS

10/576,492

CN Methanone, [4-(4-chlorophenoxy)-3-[(methylamino)methyl]phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

RN 1000392-01-7 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(3-fluorophenoxy)-3-[(methylamino)methyl]phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} O & CH_2-NHMe \\ \hline \\ R & R \end{array}$$

RN 1000392-02-8 CAPLUS

CN Methanone, [3-[(cyclopropylamino)methyl]-4-(3-pyridinyloxy)phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\$$

RN 1000392-03-9 CAPLUS

CN Methanone, [4-(4-chlorophenoxy)-3-[(cyclopropylamino)methyl]phenyl](4-

cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

RN 1000392-04-0 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[3-[(methylamino)methyl]-4-phenoxyphenyl]- (CA INDEX NAME)

RN 1000392-05-1 CAPLUS

CN Methanone, [4-(3-chlorophenoxy)-3-[(methylamino)methyl]phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 1000392-07-3 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-y1)[3[(methylamino)methyl]-4-[3-methyl-4-(methylthio)phenoxy]phenyl]- (CA
INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 1000392-08-4 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[3-[(methylamino)methyl]-4-[4-(methylthio)phenoxy]phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 1000392-09-5 CAPLUS

CN Methanone, [3-[(cyclopropylamino)methyl]-4-(3,4-dichlorophenoxy)phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

RN 1000392-11-9 CAPLUS

CN Methanone, [4-(3-chloro-2-fluorophenoxy)-3-[(methylamino)methyl]phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN 1000392-12-0 CAPLUS

CN Methanone, [4-(3-chloro-4-fluorophenoxy)-3-[(methylamino)methyl]phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 1000392-13-1 CAPLUS

CN Methanone, [4-(4-chloro-2-fluorophenoxy)-3-[(methylamino)methyl]phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

RN 1000392-14-2 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-y1)[3-[(methylamino)methyl]-4-[(6-methyl-3-pyridinyl)oxy]phenyl]- (CA INDEX NAME)

RN 1000392-15-3 CAPLUS

CN Benzonitrile, 4-[4-[(4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]-2-[(methylamino)methyl]phenoxy]- (CA INDEX NAME)

RN 1000392-16-4 CAPLUS

CN Methanone, [4-(4-chlorophenoxy)-3[(cyclopropylamino)methyl]phenyl][hexahydro-4-(1-methylethyl)-1H-1,4diazepin-1-yl]- (CA INDEX NAME)

RN 1000392-17-5 CAPLUS

CN Benzonitrile, 3-[4-[(4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]-2-[(methylamino)methyl]phenoxy]- (CA INDEX NAME)

RN 1000392-18-6 CAPLUS

CN Methanone, [3-[(cyclopropylamino)methyl]-4-(3,4-dichlorophenoxy)phenyl][hexahydro-4-(1-methylethyl)-1H-1,4-diazepin-1-yl]-(CA INDEX NAME)

RN 1000392-19-7 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(4-fluorophenoxy)-3-[(methylamino)methyl]phenyl]- (CA INDEX NAME)

RN 1000392-21-1 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(3-

methoxyphenoxy)-3-[(methylamino)methyl]phenyl]- (CA INDEX NAME)

RN 1000392-22-2 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[3[(methylamino)methyl]-4-[4-[(trifluoromethyl)thio]phenoxy]phenyl]- (CA
INDEX NAME)

RN 1000392-23-3 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-y1)[3[(methylamino)methyl]-4-[2-(trifluoromethoxy)phenoxy]phenyl]- (CA INDEX NAME)

RN 1000392-24-4 CAPLUS

CN Benzonitrile, 2-[4-[(4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]-2-[(methylamino)methyl]phenoxy]- (CA INDEX NAME)

RN 1000392-25-5 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[3-[(methylamino)methyl]-4-[2-(trifluoromethyl)phenoxy]phenyl]- (CA INDEX NAME)

RN 1000392-26-6 CAPLUS

CN Methanone, [4-[4-chloro-3-(trifluoromethyl)phenoxy]-3[(methylamino)methyl]phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)(CA INDEX NAME)

RN 1000392-27-7 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1, 4-diazepin-1-yl) [4-(2,3-difluorophenoxy)-3-[(methylamino)methyl]phenyl]- (CA INDEX NAME)

10/576,492

$$\begin{array}{c|c} & & & & \\ & &$$

RN 1000392-28-8 CAPLUS

CN Methanone, [4-(2-chloro-4-fluorophenoxy)-3-[(methylamino)methyl]phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

RN 1000392-29-9 CAPLUS

CN Methanone, [4-(4-chlorophenoxy)-3[(cyclopropylmethylamino)methyl]phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

RN 1000392-30-2 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(2,3-dichlorophenoxy)-3-[(methylamino)methyl]phenyl]- (CA INDEX NAME)

RN 1000392-31-3 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-y1)[3[(dimethylamino)methyl]-4-[(6-methyl-3-pyridinyl)oxy]phenyl]- (CA INDEX NAME)

RN 1000392-32-4 CAPLUS

CN Methanone, [4-[(4-chlorophenyl)thio]-3-[(methylamino)methyl]phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

10/576,492

RN 1000392-33-5 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[3-[(methylamino)methyl]-4-(2-pyridinylthio)phenyl]- (CA INDEX NAME)

RN 1000392-34-6 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1, 4-diazepin-1-yl)[3-[(methylamino)methyl]-4-(2-pyridinyloxy)phenyl]- (CA INDEX NAME)

RN 1000392-35-7 CAPLUS

CN Methanone, [4-[(cyclopropylamino)methyl]-3-(3-pyridinyloxy)phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 1000392-36-8 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(1-piperidinylmethyl)-3-(3-pyridinyloxy)phenyl]- (CA INDEX NAME)

RN 1000392-37-9 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1, 4-diazepin-1-yl) [4-[(3,4-dichlorophenyl)methoxy]-3-[(methylamino)methyl]phenyl]- (CA INDEX NAME)

RN 1000392-42-6 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[3[(methylamino)methyl]-4-[[4-(trifluoromethyl)-2-pyridinyl]thio]phenyl](CA INDEX NAME)

RN 1000392-43-7 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(3,4-dichlorophenoxy)-3-[(methylamino)methyl]phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{O} & \text{CH}_2\text{--}\text{NHMe} \\ \hline \\ \text{R} & \end{array}$$

RN 1000392-46-0 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(4-morpholinylmethyl)-3-(3-pyridinyloxy)phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 1000392-47-1 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[3-(3,4-dichlorophenoxy)-4-[(methylamino)methyl]phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & CH_2-NHMe \\ \hline & & & \\ & & & \\ & & & \\ \end{array}$$

RN 1000392-49-3 CAPLUS

CN Methanone, [4-[[bis(2-methoxyethyl)amino]methyl]-3-

(phenylmethoxy)phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

IT 1000392-60-8P 1000392-64-2P 1000392-67-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted aminomethyl benzamides as histamine H3 receptor and serotonin transporter modulators for treating histamine H3 receptor- and serotonin-mediated diseases)

RN 1000392-60-8 CAPLUS

CN Carbamic acid, N-[[5-[(4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]-2-(3,4-dichlorophenoxy)phenyl]methyl]-N-methyl-,
1,1-dimethylethyl ester (CA INDEX NAME)

RN 1000392-64-2 CAPLUS

CN Carbamic acid, N-cyclopropyl-N-[[4-[(4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]-2-(3-pyridinyloxy)phenyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ &$$

RN 1000392-67-5 CAPLUS

CN Carbamic acid, N-[[5-[(4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]-2-[(3,4-dichlorophenyl)methoxy]phenyl]methyl]-N-methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

$$\begin{array}{c|c} \textbf{R} & \textbf{CH}_2-\textbf{N-C-OBu-t} \\ & | & | \\ & \textbf{Me O} \end{array}$$

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:10101 CAPLUS

DOCUMENT NUMBER: 148:100641

TITLE: Preparation of substituted benzamide modulators of the

histamine H3 receptor

INVENTOR(S): Allison, Brett D.; Carruthers, Nicholas I.; Letavic,

Michael A.; Santillan, Alejandro, Jr.; Shah,

Chandravadan R.

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 64 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND DATE | APPL | ICATION NO. | DATE | | | |
|-----------------------|---------------|-------------------|----------------------------|-----------------|--|--|--|
| WO 2008002816 | A1 2008 | 0103 WO 2 | 007-US71732 | 20070621 | | | |
| W: AE, AG, AL | , AM, AT, AU, | AZ, BA, BB, | BG, BH, BR, | BW, BY, BZ, CA, | | | |
| CH, CN, CC | CR, CU, CZ, | DE, DK, DM, | DO, DZ, EC, | EE, EG, ES, FI, | | | |
| GB, GD, GE | GH, GM, GT, | HN, HR, HU, | ID, IL, IN, | IS, JP, KE, KG, | | | |
| KM, KN, KP | , KR, KZ, LA, | LC, LK, LR, | LS, LT, LU, | LY, MA, MD, ME, | | | |
| MG, MK, MN | , MW, MX, MY, | MZ, NA, NG, | NI, NO, NZ, | OM, PG, PH, PL, | | | |
| PT, RO, RS | , RU, SC, SD, | SE, SG, SK, | SL, SM, SV, | SY, TJ, TM, TN, | | | |
| TR, TT, TZ | , UA, UG, US, | UZ, VC, VN, | ZA, ZM, ZW | | | | |
| RW: AT, BE, BG | CH, CY, CZ, | DE, DK, EE, | ES, FI, FR, | GB, GR, HU, IE, | | | |
| IS, IT, LT | LU, LV, MC, | MT, NL, PL, | PT, RO, SE, | SI, SK, TR, BF, | | | |
| BJ, CF, CG | CI, CM, GA, | GN, GQ, GW, | ML, MR, NE, | SN, TD, TG, BW, | | | |
| GH, GM, KE | LS, MW, MZ, | NA, SD, SL, | SZ, TZ, UG, | ZM, ZW, AM, AZ, | | | |
| | , MD, RU, TJ, | | | | | | |
| AU 2007265238 | A1 2008 | 0103 AU 2 | 007-265238 | 20070621 | | | |
| CA 2656072 | A1 2008 | 0103 CA 2 | 007-2656072 | 20070621 | | | |
| US 20080045507 | | | | | | | |
| EP 2038269 | A1 2009 | 0325 E P 2 | 007-812229 | 20070621 | | | |
| R: AT, BE, BG | CH, CY, CZ, | DE, DK, EE, | ES, FI, FR, | GB, GR, HU, IE, | | | |
| IS, IT, LI | , LT, LU, LV, | MC, MT, NL, | PL, PT, RO, | SE, SI, SK, TR, | | | |
| AL, BA, HR | , MK, RS | | | | | | |
| CN 101511807 | A 2009 | 0819 CN 2 | 007-80032144 | 20090227 | | | |
| RIORITY APPLN. INFO.: | | | 006-806164P 007-US71732 | | | | |
| HER SOURCE(S): | | | | | | | |

GΙ

$$\begin{bmatrix} 0 \\ N \\ R^2 \\ R^3 \end{bmatrix}$$

AB The title compds. I [R1 = H, alkyl, monocyclic cycloalkyl, Ph; R2 = H or Me; or R1 and R2 taken together form monocyclic cycloalkyl; R3 = H, OH, Me; or when R1 is not H or Ph, R2 and R3 taken together form a carbonyl; q = 1-2; R4 = alkyl, alkenyl, cycloalkyl, etc.; with the proviso] that are histamine H3 receptor modulators useful in the treatment of histamine H3 receptor-mediated diseases, were prepared E.g., a multi-step synthesis of II, starting with 4-carboxybenzaldehyde, was given. Exemplified compds. I were tested for binding to the cloned human and rat H3 receptors. For example, II showed Ki of 7 nM in the human H3 receptor binding assay. Pharmaceutical compns. comprising the compound I alone or in combination with other therapeutic agent were disclosed.

ΙT 1000404-73-8P 1000404-75-0P 1000404-86-3P 1000404-87-4P 1000404-88-5P 1000404-89-6P 1000404-90-9P 1000404-94-3P 1000404-95-4P 1000404-96-5P 1000404-97-6P 1000404-98-7P 1000404-99-8P 1000405-10-6P 1000405-11-7P 1000405-13-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted benzamides as histamine H3 receptor modulators for treating histamine H3 receptor-mediated diseases)

RN 1000404-73-8 CAPLUS

CN Methanone, [4-(cyclohexylhydroxymethyl)phenyl][hexahydro-4-(1-methylethyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

RN 1000404-75-0 CAPLUS

CN Methanone, [4-(cyclohexylcarbonyl)phenyl][hexahydro-4-(1-methylethyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

RN 1000404-86-3 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(1-hydroxypropyl)phenyl]- (CA INDEX NAME)

RN 1000404-87-4 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(cyclohexylhydroxymethyl)phenyl]- (CA INDEX NAME)

RN 1000404-88-5 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(hydroxyphenylmethyl)phenyl]- (CA INDEX NAME)

RN 1000404-89-6 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(1-hydroxy-2-methylpropyl)phenyl]- (CA INDEX NAME)

RN 1000404-90-9 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(hydroxymethyl)phenyl]- (CA INDEX NAME)

RN 1000404-94-3 CAPLUS

CN Methanone, [4-(cyclohexylhydroxymethyl)phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

RN 1000404-95-4 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(hydroxymethyl)phenyl]- (CA INDEX NAME)

RN 1000404-96-5 CAPLUS

CN Methanone, [4-(cyclohexylcarbonyl)phenyl](4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

RN 1000404-97-6 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(hydroxyphenylmethyl)phenyl]- (CA INDEX NAME)

RN 1000404-98-7 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(1-hydroxypropyl)phenyl]- (CA INDEX NAME)

RN 1000404-99-8 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(1-hydroxy-2-methylpropyl)phenyl]- (CA INDEX NAME)

RN 1000405-10-6 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(1-hydroxycyclohexyl)phenyl]- (CA INDEX NAME)

RN 1000405-11-7 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(1-hydroxycyclopentyl)phenyl]- (CA INDEX NAME)

RN 1000405-13-9 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)[4-(1-hydroxycycloheptyl)phenyl]- (CA INDEX NAME)

IT 1000405-22-0P 1000405-24-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted benzamides as histamine H3 receptor modulators for treating histamine H3 receptor-mediated diseases)

RN 1000405-22-0 CAPLUS

CN Benzaldehyde, 4-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]- (CA INDEX NAME)

RN 1000405-24-2 CAPLUS

CN Benzaldehyde, 4-[(4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]- (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:1396423 CAPLUS

DOCUMENT NUMBER: 148:55081

TITLE: Preparation of pyridinone and pyridazinone derivatives

as inhibitors of poly(adp-ribose)polymerase (parp)
INVENTOR(S):

Jones, Philip; Kinzel, Olaf; Pescatore, Giovanna;
Llauger Bufi, Laura; Schultz-Fademrecht, Carsten;

Ferrigno, Federica

PATENT ASSIGNEE(S): Istituto di Ricerche di Biologia Molecolare P.

Angeletti SpA, Italy PCT Int. Appl., 101 pp.

SOURCE: PCT Int. Appl CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA: | TENT | KIND DATE | | | | | APPL | ICAT | | DATE | | | | | | | |
|----------------|-------|----------------|------|-----|--------------------------|---------------------------|------|------|------|------|----------|------|----------|-----|-----|------|-----|
| | | | | | A2 2007120 A3 2008080 | | | | | WO 2 | 007- | | 20070525 | | | | |
| | W: | V: AE, AG, AL, | | | AM, | ΑT, | AU, | ΑZ, | BA, | BB, | BG, | BH, | BR, | BW, | BY, | BZ, | CA, |
| | | | | | | | CZ, | | | | | | | | | | |
| | | GD, | GE. | GH, | GM, | GT, | HN, | HR. | HU, | ID, | IL. | IN. | IS, | JP, | KE. | KG. | KM, |
| | | | • | • | • | • | LC, | • | • | • | • | • | • | • | • | • | • |
| | | • | | | | • | NA, | | | | • | | • | • | | • | • |
| | | | | | | | SG, | | | | | | | | | | |
| | | | | | | | VC, | | | | | | · | • | • | · | |
| | RW: | ΑT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HU, | IE, |
| | | IS, | IT, | LT, | LU, | LV, | MC, | MT, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR, | BF, |
| | | ВJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | NE, | SN, | TD, | TG, | BW, |
| | | GH, | GM, | ΚE, | LS, | MW, | MZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | AZ, |
| | | BY, | KG, | KΖ, | MD, | RU, | ТJ, | TM, | ΑP, | EA, | EP, | OA | | | | | |
| ΑU | 2007 | 2668 | 36 | | A1 | | 2007 | 1206 | | AU 2 | 007 - 3 | 2668 | 36 | | 2 | 0070 | 525 |
| | 2653 | | | | | | | | | | | | | | | | |
| EΡ | 2029 | 551 | | | A2 | 2 20090304 EP 2007-733716 | | | | | | | | | | | |
| | R: | ΑT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HU, | IE, |
| | | IS, | ΙΤ, | LI, | LT, | LU, | LV, | MC, | MT, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR, |
| | | AL, | BA, | HR, | MK, | RS | | | | | | | | | | | |
| US | 2009 | 0176 | 765 | | A1 | | 2009 | 0709 | | US 2 | 008- | 2275 | 13 | | 2 | 0081 | 119 |
| ΙN | 2008 | DN09 | 794 | | Α | | 2009 | 0320 | | | 0.08 - 1 | | _ | | | | |
| MX | 2008 | 0150 | 14 | | Α | | 2009 | 0417 | | | 008- | | | | _ | 0081 | |
| KR 2009015092 | | | | | Α | | 2009 | 0211 | | | 008- | | | | | | |
| CN 101501006 | | | | | | | | | 1 | CN 2 | 007- | 8002 | 0136 | | 2 | 0081 | 201 |
| | 2008 | | | | А | | 2009 | 0225 | | NO 2 | 008 - | 5397 | | | 2 | 0081 | 229 |
| ORIT: | Y APP | LN. | INFO | .: | | | | | | | 006- | | | | | | |
| HER SOURCE(S): | | | | | | | | | | | 007- | | | | W 2 | 0070 | 525 |
| ER SO | OURCE | (S): | | | CAS | REAC | T 14 | 8:55 | 081; | MAR | PAT | 148: | 55081 | 1 | | | |

GΙ

$$(R^{1})_{m}$$

$$(R^{1})_{n}$$

$$(R^{1})_{n}$$

$$(R^{2})_{p}$$

$$(R^{2})_{p}$$

$$(R^{2})_{p}$$

Title compound I [R1 independently = alkyl, haloalkyl, halo or CN; m and n AΒ independently = 0 or 1; R2 independently = OH, halo, CN, alkyl, etc.; p = 0-3; R5 = H, OH, CN, alkyl, etc.; X1 = N or CH; X2 = (CH2)c(CO)d(NR3)e(Z=O)f(O)g(CH2)h(NR4)i; where R3 and R4 independently = H or alkyl; Z = C or SO; c and h independently = 0-6; d, e, f, g, and i independently = 0 or 1], and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of poly(adp-ribose)polymerase (parp). Thus, e.g., the trifluoroacetate salt of II was prepared by acetylation of $4-\{5-[(5-\text{ethyl}-6-\text{oxo}-1,6-\text{dihydropyridazin}-3-\text{yl})\text{methyl}]-2-\text{fluorobenzoyl}\}-$ 1,4-diazepane trifluoroacetate salt (preparation given). The exemplified compds. described and tested by PARP-1 SPA assay were found to have an IC50 value of less than 5 μM . I should prove useful for the treatment of cancer, inflammatory diseases, reperfusion injuries, ischemic conditions, stroke, renal failure, cardiovascular diseases, vascular diseases other than cardiovascular diseases, diabetes mellitus, neurodegenerative diseases, retroviral infections, retinal damage, skin senescence and UV-induced skin damage, and as chemo- or radiosensitizers for cancer treatment.

IT 959840-05-2P 959840-06-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridinone and pyridazinone derivs. as inhibitors of poly(adp-ribose)polymerase)

RN 959840-05-2 CAPLUS

CN 3(2H)-Pyridazinone, 6-[[3-[[4-(cyclopentylcarbonyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-4-fluorophenyl]methyl]-4,5-dimethyl- (CA INDEX NAME)

RN 959840-06-3 CAPLUS

CN 3(2H)-Pyridazinone, 6-[[3-[[4-(cyclopentylcarbonyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-4-fluorophenyl]methyl]-4-ethyl- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \text{Et} \\ & & & \\$$

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L16 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:150717 CAPLUS

DOCUMENT NUMBER: 146:229372

TITLE: Preparation of imidazolyl-pyrimidine compounds as CDK2

inhibitors

INVENTOR(S): Andrews, David; Finlay, Maurice Raymond; Green, Clive;

Jones, Clifford

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca Uk Limited

SOURCE: PCT Int. Appl., 159pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA: | TENT | NO. | | | KIND DATE | | | | APPI | LICAT | ION : | DATE | | | | | |
|---------|----------------|----------|----------|------|-----------|-----------------|-------------------|-------|------|-------|----------|------|----------------------|----------------------|------|------|-----|
| WO | 2007 | 0150 | 64 | | | 2007 | 0208 | | WO 2 | 2006- | GB28 | 01 | | 2 | 0060 | 727 | |
| | W: | CN, | CO, | CR, | CU, | CZ, | AU, DE, HU, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, |
| | | • | • | • | • | | LR, | | | | | • | • | • | • | • | • |
| | | SC, | SD, | SE, | SG, | SK, | SL, | SM, | • | , | • | • | • | • | • | • | • |
| | RW: | | | | | | CZ, MC, | | | | | | | | | | |
| | | CF, | CG, | CI, | CM, | GA, | GN, NA, | GQ, | GW, | ML, | MR, | ΝE, | SN, | TD, | TG, | BW, | GH, |
| | | | | | RU, | | TM | | | | | | | · | · | · | · |
| | 2006 | | 33 | A1 | | 2007 | 0208 | | AU 2 | 2006- | 2747 | 33 | | 2 | 0060 | | |
| _ | 2617 | A1 | | 2007 | 0208 | | CA 2 | 2006- | 2617 | 170 | | 2 | | | | | |
| EP | 1912 | _ | | | A1 | | 2008 | | | | | | | | | 0060 | |
| | R: | | | | | | CZ, | | | | | | | | | | |
| | 2000 | | | | | | LV, | | | | | | | | | | |
| | 2008 | | | | | | | | | JP 2 | 2008- | 5142 | | 2 | 0060 | /2/ | |
| | 4278 | | | | B2 | | 2009 | | | NTO (| 2000 | C 1 | | | ^ | 0000 | 101 |
| | 2008 2008 | | | | | | | | | | 2008- | | 20080104 20080104 | | | | |
| | 2008 | | | | A | | | | | | | | | | | | |
| | 2008 | | 40 50 | | Α. 7\ | | 2008 | | | | | | | 20080129 20080226 | | | |
| | 1012 | | J 0 1 | | A | | 2008 | | | | 2006- | | | | | 0000 | |
| | | | 906 | | Δ1 | | | | | | 2008- | | | | | 0080 | |
| JP. | 2008 2009 | 1379 | 90 | | A | | 2009 | | | | 2009- | | | | | 0090 | |
| IORIT | | | | | | | 2003 | 0020 | | | 2005- | | | ; | _ | 0050 | |
| | | | | • • | | | | | | GB 2 | 2005- | 2028 | 1 | - | | 0051 | |
| | | | | | | | | | | GB 2 | 2005- | 2601 | - 5 | 3 | | 0051 | |
| | | | | | | GB 2 | 2006- | 8371 | - | | | 0060 | | | | | |
| | | | | | | | | | | | 2008- | | | | | 0060 | _ |
| | | | | | | | | 2006- | | | | | 0060 | | | | |
| THER SO | HER SOURCE(S): | | | | | MARPAT 146:2293 | | | | | | | | | | | |

OTHER SOURCE(S): MARPAT 146:229372

GI

Title compds. I [R1 = Et, Pr, iso-Pr, etc.; R2 = Me, Et, iso-Pr, etc.; R3 AB = H or halo; R4 = H, ethynyl, halo, etc.; ring A = nitrogen-linked saturated ring which optionally contains an addnl. nitrogen, oxygen or sulfur atom; wherein 2 atoms of ring A, when ring A is a nitrogen-linked saturated ring, may optionally be connected by a one or two atom bridge.; and wherein if ring A contains an addnl. nitrogen atom that nitrogen may be optionally substituted by R7.; R5 = substituent on carbon and selected from halo, cyano, hydroxy, etc.; R7 = alkyl, alkanoyl, alkylsulfonyl, etc.; n = 0-2], pharmaceutically acceptable salts or in-vivo hydrolyzable ethers thereof were prepared For example, Pd(OAc)2 catalyzed coupling reaction of 5-fluoro-4-(3-isopropyl-2-methyl-3H-imidazol-4-yl)pyrimidin-2-ylamine, e.g., prepared from (2E)-3-dimethylamino-1-(1-isopropyl-2-methyl-1H-imidazol-5-yl)prop-2-en-1-one in 2 steps, with (4-iodophenyl)-morpholin-4-yl-methanone afforded compound II [X = F]. CDK2 (cyclin-dependent kinase 2) inhibition assays, compound II [X = H] exhibited the IC50 value of 3 nM. Compds. I are claimed useful for the treatment of proliferative disorders.

IT 924641-32-7P 924641-52-1P 924641-54-3P 924641-58-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of imidazolyl-pyrimidine compds. as CDK2 inhibitors for treatment of proliferative disorders)

RN 924641-32-7 CAPLUS

CN Methanone, [4-[[4-(1-cyclopentyl-2-methyl-1H-imidazol-5-yl)-2-pyrimidinyl]amino]phenyl][hexahydro-4-(1-methylethyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

RN 924641-52-1 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1, 4-diazepin-1-yl) [4-[[4-[2-methyl-1-(1-methylethyl)-1H-imidazol-5-yl]-2-pyrimidinyl]amino]phenyl]- (CA INDEX NAME)

RN 924641-54-3 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-[[4-[2-methyl-1-(1-methylethyl)-1H-imidazol-5-yl]-2-pyrimidinyl]amino]phenyl]- (CA INDEX NAME)

RN 924641-58-7 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-[[5-fluoro-4-[2-methyl-1-(1-methylethyl)-1H-imidazol-5-yl]-2-pyrimidinyl]amino]phenyl](CA INDEX NAME)

IT 924643-15-2P, (4-Cyclopropyl-1,4-diazepan-1-yl)(4iodophenyl)methanone 924643-16-3P,
 (4-Cyclobutyl-1,4-diazepan-1-yl)(4-iodophenyl)methanone

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of imidazolyl-pyrimidine compds. as CDK2 inhibitors for treatment of proliferative disorders)

RN 924643-15-2 CAPLUS

CN Methanone, (4-cyclopropylhexahydro-1H-1,4-diazepin-1-yl)(4-iodophenyl)- (CA INDEX NAME)

RN 924643-16-3 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)(4-iodophenyl)- (CA INDEX NAME)

REFERENCE COUNT:

4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:1119177 CAPLUS

DOCUMENT NUMBER: 145:471561

TITLE: Diarylmethylpiperazines as $\mu-$ and $\delta-$ opioid receptor modulators and their preparation,

pharmaceutical compositions and method of use thereof INVENTOR(S): Jan, Shyi-Tai; Chang, Kwen-Jen; Biciunas, Kestutis P.;

Ma, Xin

PATENT ASSIGNEE(S): Ardent Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 164pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA | TENT | NO. | | | KIND DATE | | | • | APPL | ICAT | | DATE | | | | | |
|----------------------------|--|---|---|---|---|--|--|--|--|--|---|------------------------------------|---------------------------------|---|---|---|---|
| | 2006 2006 | | | | | | | | | 0060 | 414 | | | | | | |
| | W: | AE, CN, GE, KZ, MZ, SG, VN, AT, IS, | AG, CO, GH, LC, NA, SK, YU, BE, IT, | AL, CR, GM, LK, NG, SL, ZA, BG, LT, | AM, CU, HR, LR, NI, SM, ZM, CH, LU, | AT, CZ, HU, LS, NO, SY, ZW CY, LV, | AU, DE, ID, LT, NZ, TJ, | AZ, DK, IL, LU, OM, TM, | BA, DM, IN, LV, PG, TN, | DZ, IS, LY, PH, TR, | BG, EC, JP, MA, PL, TT, ES, RO, MR, | EE, KE, MD, PT, TZ, | EG, KG, MG, RO, UA, | ES, KM, MK, RU, UG, GB, SK, | FI, KN, MN, SC, US, GR, TR, | GB, KP, MW, SD, UZ, HU, BF, | GD, KR, MX, SE, VC, IE, BJ, |
| | | GM, | KE, | LS, | | MZ, | NA, | | | | TZ, | | | | | | |
| AU CA US EP JP | 2008 | 2366 677 0043 315 AT, IS, 5466 | 22 028 BE, IT, 38 | BG, LI, | A1 A1 A2 CH, LT, | CY, LU, | 2006 2006 2007 2008 CZ, LV, 2008 | 1026 1026 0222 0109 DE, MC, 1225 | DK, NL, | CA 2 US 2 EP 2 EE, PL, JP 2 | 006- 006- 006- ES, PT, | 2643 4046 7502 FI, RO, | 677 32 23 FR, SE, | GB, SI, | 2 2 2 GR, SK, | 0060 0060 0060 HU, TR | 414 414 414 IE, |
| CN PRIORIT | IN 2007DN08715 CN 101198330 RIORITY APPLN. INFO.: IHER SOURCE(S): | | | | | | 2008 | 0611 | | CN 2 US 2 WO 2 | 006- 005- 006- |] | 20071214 P 20050414 | | | | |

^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Diarylmethylpiperazine compds. of formula I are described, which are useful as mu and/or δ receptor opioid compds., without central side effects. Pharmaceutical compns. containing such compds. are variously useful for peripheral or non-centrally mediated indications, including peripherally mediated and neuropathic pain, urogenital tract disorders,

overactive bladder, urinary incontinence, sexual disorders, premature ejaculation, cough, lung edema, cardiac disorders, cardioprotection, gastro-intestinal disorders, diarrhea, irritable bowl syndrome, functional distention, immuno-modulation and anti-tumor activity. Compds. of formula I wherein Z is H, O(CH2)mCH3, and OH; m is 0 to 4; X is CO and SO2, which is in the meta or para position of the Ph ring; DL is difunctional amine liner having a nitrogen covalently bonded to the carbon or sulfur atom to the X group; Q is CH2, CH2Ar and CH2Ch2Ar, wherein the difunctional linker is covalently bonded to the terminal carbon of the Q group; Ar is disubstituted 5- or 6-membered carbocyclic and heteroarom. ring; n is 0, 1, 2, 3, 4, and 5; R1 is C1-6 alkyl, C2-6 alkenyl, C1-6 cycloalkylmethyl, C5-10 aryl-C1-4 alkyl, (halo)benzyl, and carboxybenzyl; R2 is H and salts thereof are claimed. Example compound II was prepared by amidation of 3-[(R)-((2S,5R)-4-allyl-2,5-dimethylpiperazin-1-yl)(3hydroxyphenyl)methyl]benzoic acid with homopiperazine. All the invention compds. were evaluated for their in vitro opioid receptor affinity (data given).

IT 913643-81-9P 913643-82-0P 913643-84-2P 913643-86-4P 913643-87-5P 913643-88-6P 913643-94-4P 913644-05-0P 913644-12-9P 913644-13-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of diarylmethylpiperazines as $\mu-$ and $\delta-$ opioid receptors modulating compds. useful in treatment of diseases)

RN 913643-81-9 CAPLUS

CN 1H-1,4-Diazepine-1-acetic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 913643-82-0 CAPLUS

CN 1H-1, 4-Diazepine-1-acetic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro- (CA INDEX NAME)

RN 913643-84-2 CAPLUS

CN 1H-1,4-Diazepine-1-propanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 913643-86-4 CAPLUS

CN 1H-1,4-Diazepine-1-propanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro- (CA INDEX NAME)

RN 913643-87-5 CAPLUS

CN 1H-1,4-Diazepine-1-butanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 913643-88-6 CAPLUS

CN 1H-1, 4-Diazepine-1-butanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro- (CA INDEX NAME)

RN 913643-94-4 CAPLUS

CN 1H-1,4-Diazepine-1-pentanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 913643-96-6 CAPLUS

CN 1H-1,4-Diazepine-1-pentanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro- (CA INDEX NAME)

$$Me$$
 R
 N
 S
 Me
 R
 N
 S
 Me
 Me
 R
 N
 S
 Me

RN 913644-04-9 CAPLUS

CN 1H-1,4-Diazepine-1-hexanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 913644-05-0 CAPLUS

CN 1H-1, 4-Diazepine-1-hexanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro- (CA INDEX NAME)

RN 913644-12-9 CAPLUS

CN 1H-1,4-Diazepine-1-heptanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 913644-13-0 CAPLUS

CN 1H-1,4-Diazepine-1-heptanoic acid, 4-[3-[(R)-[(2S,5R)-4-(cyclopropylmethyl)-2,5-dimethyl-1-piperazinyl](3-hydroxyphenyl)methyl]benzoyl]hexahydro- (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:606105 CAPLUS

DOCUMENT NUMBER: 145:83375

TITLE: Preparation of pyrazolo[1,5-a]pyrimidine derivatives

as adenosine A2a receptor antagonists

INVENTOR(S): Clasby, Martin C.; Chackalamannil, Samuel; Neustadt,

Bernard R.; Gao, Xiaobang

PATENT ASSIGNEE(S): Schering Corp., USA

SOURCE: U.S. Pat. Appl. Publ., 79 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA | TENT | NO. | KIND DATE | | | | | | ICAT | | DATE | | | | | | | |
|----------|-------------------------------------|-------|-----------|-----|-------------|---------|--------------------------------------|------|----------------|------------------------------------|------|------|-----|------|------------|------|-----|--|
| US | 2006 | 0135 | 526 | | A1 | | 2006 | 0622 | | US 2 | | | 2 | 0051 | 219 | | | |
| CA | 2591 | 125 | | | A1 | | 2006 | 0629 | 1 | | | | | 0051 | 219 | | | |
| | | | | | A2 20060629 | | | | | | | | | | 20051219 | | | |
| | 2006 | | | | | | | | | | | | | | | | | |
| | W: | ΑE, | AG, | AL, | AM, | ΑT, | AU, | AZ, | BA, | BB, | BG, | BR, | BW, | BY, | BZ, | CA, | CH, | |
| | | | | | | | DE, | | | | | | | | | | | |
| | | GE, | GH, | GM, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KM, | KN, | KP, | KR, | |
| | | KΖ, | LC, | LK, | LR, | LS, | LT, | LU, | LV, | LY, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | |
| | | MZ, | NA, | NG, | ΝI, | NO, | NΖ, | OM, | PG, | PH, | PL, | PT, | RO, | RU, | SC, | SD, | SE, | |
| | | SG, | SK, | SL, | SM, | SY, | ТJ, | TM, | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UZ, | VC, | |
| | | VN, | YU, | ZA, | ZM, | ZW | | | | | | | | | | | | |
| | RW: | AT, | BE, | ВG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FΙ, | FR, | GB, | GR, | HU, | IE, | |
| | | IS, | ΙΤ, | LT, | LU, | LV, | MC, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR, | BF, | ВJ, | |
| | | | • | | | | GN, | ~ . | | | , | • | • | | | | | |
| | | GM, | KΕ, | LS, | MW, | MZ, | NΑ, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | ΑZ, | BY, | |
| | | | KΖ, | | | | | | | | | | | | | | | |
| | | | | | | | | | EP 2005-854388 | | | | | | 20051219 | | | |
| EP | 1836 | | | | | | | | | | | | | | | | | |
| | R: | | | | | | CZ, | | | | | | • | • | • | | | |
| | | | | | | LU, | LV, | MC, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR, | AL, | |
| | | | HR, | | | | | | | _ | | | | | | | | |
| JP | 2008 | 5243 | 30 | | T | | 2008 | 0710 | 1 | JP 2 | 007- | 5483 | 34 | | 2 | 0051 | | |
| AT | AT 433454 | | | | | | 2009 | 0615 | | AT 2 | 005- | 8543 | 88 | | 2 | 0051 | 219 | |
| MX | MX 2007007604 CN 101119998 | | | | | | 2007 | 0802 | ŀ | MX 2 | 007- | 7604 | | | 2 | 0070 | 621 | |
| | CN 101119998 PRIORITY APPLN. INFO.: | | | | | | 2008 | 0206 | | | | | | | | | | |
| PRIORIT | Y APP | LN. | TNF.O | .: | | | | | | US 2004-638028P WO 2005-US45658 | | | | | | | | |
| OM1100 C | 011D C = | , a \ | | | 07.0 | D D 3 ~ | m 1 4 | - A2 | | | | | | | W 20051219 | | | |
| OTHER S | | | | | | | CASREACT 145:83375; MARPAT 145:83375 | | | | | | | | | | | |

GI

$$R^2$$
 R^2
 R^2
 R^3
 R^4 R^4

AΒ Compds. having the structural formula [I; A = alkylene, (un)substitutedarylene, cycloalkylene or heteroaryldiyl; X = CO, SO2; R1 = alkyl, cycloalkyl; R2 = H, halo, cyano; R3 = H, alkyl; R4 = H, alkyl, alkoxy, hydroxyalkyl, aminoalkyl-, cycloalkyl, heterocycloalkyl, heterocycloalkyl substituted by alkyl, each (un)substituted arylalkyl or heteroarylalkyl; or R3 and R4 form an (un)substituted 5-7 membered ring optionally comprising an addnl. heteroatom ring member; R7 = alkyl, cycloalkyl, halo, morpholinyl, each (un)substituted Ph or heteroaryl, piperazinyl, or azacycloalkyl] are prepared These compds. are adenosine A2a receptor antagonists and useful in the treatment of central nervous system diseases, stroke, depression, cognitive diseases, neurodegenerative diseases (in particular Parkinson's disease), senile dementia, psychoses, attention deficit disorder, extrapyramidal syndrome, dystonia, restless leg syndrome, periodic limb movement in sleep. They are used alone or in combination with other agents (e.g. L-DOPA) for treating Parkinson's disease. Thus, 90 mg 4-amino-N, N-dimethylbenzenesulfonamide was added to a solution of 100 mg 7-chloro-2-methyl-5-phenylprazolo[1,5-a]pyrimidine in 4 mL DMF followed by adding 92 mg potassium tert-butoxide and the resulting mixture was stirred for 3 h to give 45 mg pyrazolo[1,5-a]pyrimidine derivative (II). The compds. I showed the binding affinity to human adenosine A2A receptor with Ki of .apprx.0.1 to .apprx.1,800 nM. ΙT

893446-40-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of pyrazolo[1,5-a]pyrimidine derivs. as adenosine A2a receptor antagonists)

893446-40-7 CAPLUS RN

Methanone, [4-[(2-cyclopropyl-5-phenylpyrazolo[1,5-a]pyrimidin-7-CN yl)amino]phenyl][hexahydro-4-(phenylmethyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

SOURCE:

L16 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:395292 CAPLUS

DOCUMENT NUMBER: 142:430314
TITLE: Preparation of

(1H-1,4-diazepan-1-yl)(phenyl)methanones as histamine H3 functional antagonists for treating neurological

disorders

INVENTOR(S): Bruton, Gordon; Huxley, Anthony; Orlek, Barry Sidney;

Rana, Kishore Kalidas Glaxo Group Limited, UK PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT ASSIGNEE(S):

| PF | ATENT | NO. | | | KIN | D | DATE | | APPLICATION NO. | | | | | | DATE | | | |
|---------|----------------|------------|------|------|------|----------|------|------|-----------------|------|------|------------|----------|----------|------|------|-----|--|
| WC | 2005 | 2005040144 | | | | A1 20050 | | | | WO 2 | 004- | | 20041014 | | | | | |
| | W: | ΑE, | AG, | AL, | AM, | ΑT, | AU, | AZ, | BA, | BB, | BG, | BR, | BW, | BY, | BZ, | CA, | CH, | |
| | | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, | |
| | | GE, | GH, | GM, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | ΚE, | KG, | KP, | KR, | KΖ, | LC, | |
| | | LK, | LR, | LS, | LT, | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NA, | NI, | |
| | | NO, | NZ, | OM, | PG, | PH, | PL, | PT, | RO, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SY, | |
| | | ТJ, | TM, | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UΖ, | VC, | VN, | YU, | ZA, | ZM, | ZW | |
| | RW: | BW, | GH, | GM, | ΚE, | LS, | MW, | MZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | |
| | | AZ, | BY, | KG, | KΖ, | MD, | RU, | ТJ, | TM, | AT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | |
| | | EE, | ES, | FI, | FR, | GB, | GR, | HU, | ΙE, | IT, | LU, | MC, | NL, | PL, | PT, | RO, | SE, | |
| | | SI, | SK, | TR, | BF, | ВJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | NE, | |
| | | SN, | TD, | ΤG | | | | | | | | | | | | | | |
| EF | 1675 | 838 | | | A1 | | 2006 | 0705 | | EP 2 | 004- | 7659 | 73 | 20041014 | | | | |
| | R: | AT, | BE, | CH, | DE, | DK, | ES, | FR, | GB, | GR, | ΙΤ, | LI, | LU, | NL, | SE, | MC, | PT, | |
| | | ΙE, | SI, | LT, | LV, | FI, | RO, | CY, | TR, | BG, | CZ, | EE, | HU, | PL, | SK, | HR | | |
| JE | 2007 | 5083 | 46 | | T | | 2007 | 0405 | 1 | JP 2 | 006- | 5347 | 02 | | 2 | 0041 | 014 | |
| US | US 20080045505 | | | | | | 2008 | 0221 | | US 2 | 007- | 5764 | 92 | | 2 | 0070 | 206 | |
| PRIORIT | Y APP | LN. | INFO | .: | | | | | 1 | GB 2 | 003- | 2415 | 9 | | A 2 | 0031 | 015 | |
| | | | | | | , | WO 2 | 004- | EP11 | 619 | 1 | W 20041014 | | | | | | |
| OTHER S | OURCE | CAS | REAC | T 14 | 2:43 | 0314 | ; MA | RPAT | 142 | :430 | 314 | | | | | | | |

$$R^{1-N}$$
 N
 CO
 R^{2}
 R^{2}
 R^{2}
 R^{2}

AB The present invention relates to novel diazepanyl derivs. (shown as I; variables defined below; e.g. 4'-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]-4-biphenylcarbonitrile (II)) having pharmacol. activity, processes for their preparation, to compns. containing them and to their use in the

treatment of neurol. disorders. For I: R1 = branched C3-6 alkyl, C3-5 cycloalkyl or C1-4 alkylC3-4 cycloalkyl; <math>R2 = halo, C1-6 alkyl, C1-6

GI

alkoxy, cyano, amino or trifluoromethyl; n = 0-2; R3 = X-aryl, X-heteroaryl, X-heterocyclyl, X-arylaryl, X-arylheteroaryl, X-arylheterocyclyl, X-heteroarylaryl, X-heteroarylheteroaryl, X-heteroarylheterocyclyl, X-heterocyclylaryl, X-heterocyclylheteroaryl or X-heterocyclylheterocyclyl; such that when R3 = X-piperidinyl, X-piperidinylaryl, X-piperidinylheteroaryl or X-piperidinylheterocyclyl said piperidinyl group is attached to X via a N atom; wherein R3 is attached to the Ph group of I at the 3 or 4 position; X = a bond, 0, CO, SO2, CH2O, OCH2, NR4, NR4CO or C1-6-alkyl. R4 = H or C1-6 alkyl; wherein said aryl, heteroaryl or heterocyclyl groups of R3 may be (un)substituted by ≥1 (e.g. 1, 2 or 3) halo, hydroxy, cyano, nitro, oxo, haloC1-6 alkyl, haloC1-6 alkoxy, C1-6 alkyl, C1-6 alkoxy, arylC1-6 alkoxy, C1-6 alkylthio, C1-6 alkoxyC1-6 alkyl, C3-7 cycloalkylC1-6 alkoxy, C3-7 cycloalkylcarbonyl, -COC1-6 alkyl, C1-6 alkoxycarbonyl, arylC1-6 alkyl, heteroarylC1-6-alkyl, heterocyclylC1-6 alkyl, C1-6 alkylsulfonyl, C1-6 alkylsulfinyl, C1-6 alkylsulfonyloxy, C1-6 alkylsulfonylC1-6 alkyl, arylsulfonyl, arylsulfonyloxy, arylsulfonylC1-6 alkyl, aryloxy, CO-aryl, CO-heterocyclyl, CO-heteroaryl, C1-6 alkylsulfonamidoC1-6 alkyl, C1-6 alkylamidoC1-6 alkyl, arylsulfonamido, arylaminosulfonyl, arylsulfonamidoC1-6 alkyl, arylcarboxamidoC1-6 alkyl, aroylC1-6 alkyl, arylC1-6 alkanoyl, NR15R16, NR15C0-aryl, NR15C0-heterocyclyl, NR15CO-heteroaryl, CONR15R16, NR15COR16, NR15SO2R16 or SO2NR15R16 groups, wherein R15 and R16 = independently H or C1-6 alkyl. Although the methods of preparation are not claimed, 58 example prepns. and/or characterization data sets for I are included; example prepns. for intermediates are also included. For example, II was prepared from 1-(cyclobutyl)hexahydro-1H-1,4-diazepine dihydrochloride and 4'-cyano-4-biphenylcarboxylic acid using diethylaminomethylpolystyrene, HOBT and EDC in CH2Cl2. The diazepine reactant was prepared in 2 steps starting from tert-Bu hexahydro-1H-1,4-diazepine-1-carboxylate and cyclobutanone followed by deprotection at N. The 58 example I were tested in the histamine H3 functional antagonist assay and exhibited pKb values > 8.0. Most particularly, the hydrochlorides of II, 1-[4'-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]biphenyl-4yl]ethanone, 1-cyclobutyl-4-[[4-[6-(trifluoromethyl)-3pyridinyl]phenyl]carbonyl]hexahydro-1H-1,4-diazepine, 6-[4-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-3cyanopyridine and 1-Cyclobutyl-4-[[4-(3-methyl-1,2,4-oxadiazol-5yl)phenyl]carbonyl]hexahydro-1H-1,4-diazepine exhibited pKb values >9.5. Most of the 58 example I were tested in the histamine H1 functional antagonist assay and exhibited antagonism < 7.0 pKb; most of these exhibited antagonism < 6.0 pKb. 851048-57-2P, 4'-[(4-Cyclobutylhexahydro-1H-1,4-diazepin-1yl)carbonyl]-4-biphenylcarbonitrile hydrochloride 851048-58-3P , 1-[4'-[(4-Cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]biphenyl-4yl]ethanone hydrochloride 851048-59-4P, (4-Cyclobutyl-1H-1, 4-diazepan-1-yl) (biphenyl-4-yl) methanone hydrochloride 851048-60-7P, (4-Cyclobutyl-1H-1, 4-diazepan-1-yl) (4benzoylphenyl) methanone hydrochloride 851048-61-8P, (4-Cyclobutyl-1H-1, 4-diazepan-1-yl) (4-phenoxyphenyl) methanone hydrochloride 851048-62-9P, (4-Cyclobutyl-1H-1,4-diazepan-1-yl)(4-benzyloxyphenyl)methanone 851048-63-0P, hydrochloride 1-Cyclobuty1-4-[[4-(tetrazol-1-yl)phenyl]carbonyl]hexahydro-1H-1,4diazepine hydrochloride 851048-64-1P, 1-Cyclobutyl-4-[[4-[4-(4-fluorophenyl)-1,3-thiazol-2yl]phenyl]carbonyl]hexahydro-1H-1,4-diazepine hydrochloride

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851048-65-2P, 1-Cyclobuty1-4-[[4-(1,1-dioxido-4-
thiomorpholinyl)phenyl]carbonyl]hexahydro-1H-1,4-diazepine hydrochloride
851048-67-4P, 1-Cyclobutyl-4-[[4-[6-(trifluoromethyl)-3-
pyridinyl]phenyl]carbonyl]hexahydro-1H-1,4-diazepine hydrochloride
851048-68-5P, 6-[4-[(4-Cyclobutylhexahydro-1H-1,4-diazepin-1-1]]
yl)carbonyl]phenyl]-3-cyanopyridine hydrochloride
                                                   851048-69-6P
, 5-[4-[(4-Cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-N-
methyl-2-pyridinecarboxamide hydrochloride 851048-70-9P,
5-[4-[(4-Cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-2-
cyanopyridine hydrochloride
                              851048-78-7P,
1-Cyclobutyl-4-[[4-[6-(trifluoromethyl)-3-
pyridazinyl]phenyl]carbonyl]hexahydro-1H-1,4-diazepine hydrochloride
851048-79-8P, 1-Cyclobutyl-4-[[4-[2-(trifluoromethyl)-5-
pyrimidinyl]phenyl]carbonyl]hexahydro-1H-1,4-diazepine hydrochloride
851048-80-1P, (4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4-[3-
(aminocarbonyl)phenyl]phenyl]methanone hydrochloride
851048-81-2P, (4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4-[4-cyano-3-
(trifluoromethy1)-1H-pyrazol-1-y1]pheny1]methanone hydrochloride
851048-82-3P, (4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4-[[2-oxo-5-
(trifluoromethyl)-1,2-dihydropyridin-1-yl]methyl]phenyl]methanone
hydrochloride
               851048-84-5P,
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl) [4-[(4,6-dimethylpyrimidin-2-
yl) (methyl) amino]phenyl]methanone hydrochloride
                                                 851048-85-6P,
(4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4-(4-fluorophenyl)phenyl]methanone
               851048-86-7P,
hvdrochloride
(4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4-(3-fluorophenyl)phenyl]methanone
hydrochloride
               851048-87-8P,
(4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4-(pyridin-2-yl)phenyl]methanone
              851048-88-9P,
hydrochloride
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl) [4-(pyridin-3-yl)phenyl]methanone
              851048-89-0P,
hydrochloride
(4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4-(4-cyanophenoxy)phenyl]methanone
                851048-90-3P,
hydrochloride
(4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4-(phenoxymethyl)phenyl]methanone
hydrochloride
                851048-91-4P,
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[4-(3,5-dimethylisoxazol-4-
yl)phenyl]methanone hydrochloride
                                  851048-93-6P,
(4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4-(oxazol-5-yl)phenyl]methanone
                851048-94-7P,
hvdrochloride
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[4-(2-ethyl-2H-tetrazol-5-
yl)phenyl]methanone hydrochloride
                                   851048-95-8P,
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl) [4-(pyrrol-1-yl)phenyl]methanone
                851048-96-9P,
hydrochloride
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[4-(3,5-dimethyl-1H-pyrazol-1-
yl)phenyl]methanone hydrochloride 851048-97-0P,
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[4-[(3,5-dimethyl-1H-pyrazol-1-yl)]
yl)methyl]phenyl]methanone hydrochloride
                                          851048-98-1P,
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl) [4-(morpholin-4-yl) phenyl] methanone
hydrochloride
               851049-00-8P,
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl) [3-(benzyloxy)phenyl]methanone
hydrochloride
                851049-01-9P,
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[3-[(pyridin-3-
yl)methoxy]phenyl]methanone hydrochloride
                                            851049-02-0P,
(4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[3-[(pyrazin-2-
yl)methoxy]phenyl]methanone hydrochloride
                                          851049-03-1P,
(4-Cyclobutyl-1H-1,4-diazepan-1-yl)[3-(5-methyl-1H-tetrazol-1-
yl)phenyl]methanone hydrochloride
                                   851049-04-2P,
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CN

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(4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[3-(2-oxopyrrolidin-1-
     yl)phenyl]methanone hydrochloride
                                       851049-05-3P,
     (4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[3-[[(pyridin-3-
     yl)carbonyl]amino]phenyl]methanone hydrochloride
                                                       851049-06-4P,
     (4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[3-[[(pyridin-4-
     yl)carbonyl]amino]phenyl]methanone hydrochloride
                                                       851049-07-5P,
     (4-Cyclobutyl-1H-1, 4-diazepan-1-yl) [3-(pyridin-3-yl)phenyl]methanone
     hydrochloride
                   851049-08-6P,
     (4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[4'-(oxazol-2-yl)biphenyl-4-
     yl]methanone hydrochloride
                                 851049-09-7P,
     (4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4'-(2-methyloxazol-4-yl)biphenyl-4-
     yl]methanone hydrochloride 851049-10-0P,
     (4-Cyclobutyl-1H-1,4-diazepan-1-yl)[4'-(2-methyloxazol-5-yl)biphenyl-4-
     yl]methanone hydrochloride 851049-11-1P,
     (4-Cyclobutyl-1H-1, 4-diazepan-1-yl)[4'-(5-methyl-1, 2, 4-oxadiazol-3-
     yl)biphenyl-4-yl]methanone hydrochloride
                                               851049-12-2P,
     1-Cyclobuty1-4-[[4-(1,3-oxazo1-2-y1)pheny1]carbony1]hexahydro-1H-1,4-
     diazepine hydrochloride
                             851049-19-9P,
     1-Cyclobutyl-4-[[4-(3-methyl-1, 2, 4-oxadiazol-5-
     yl)phenyl]carbonyl]hexahydro-1H-1,4-diazepine hydrochloride
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (drug candidate; preparation of (1H-1,4-diazepan-1-yl)(phenyl)methanones as
        histamine H3 functional antagonists for treating neurol. disorders)
RN
     851048-57-2 CAPLUS
     [1,1'-Biphenyl]-4-carbonitrile, 4'-[(4-cyclobutylhexahydro-1H-1,4-diazepin-
     1-yl)carbonyl]-, hydrochloride (1:1) (CA INDEX NAME)
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HC1

RN 851048-58-3 CAPLUS CN 1H-1, 4-Diazepine, 1-[(4'-acetyl[1,1'-biphenyl]-4-yl)carbonyl]-4cyclobutylhexahydro-, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 851048-59-4 CAPLUS

CN Methanone, [1,1'-biphenyl]-4-yl(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851048-60-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 851048-61-8 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)(4-phenoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851048-62-9 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-y1)[4-(phenylmethoxy)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851048-63-0 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(1H-tetrazol-1-yl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851048-64-1 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-[4-(4-fluorophenyl)-2-thiazolyl]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851048-65-2 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl) [4-(1,1-dioxido-4-thiomorpholinyl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851048-67-4 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-[6-(trifluoromethyl)-3-pyridinyl]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851048-68-5 CAPLUS

CN 3-Pyridinecarbonitrile, 6-[4-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851048-69-6 CAPLUS

CN 2-Pyridinecarboxamide, 5-[4-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-N-methyl-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851048-70-9 CAPLUS

CN 2-Pyridinecarbonitrile, 5-[4-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851048-78-7 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-[6-(trifluoromethyl)-3-pyridazinyl]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851048-79-8 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-[2-(trifluoromethyl)-5-pyrimidinyl]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851048-80-1 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, 4'-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HC1

RN 851048-81-2 CAPLUS

CN 1H-Pyrazole-4-carbonitrile, 1-[4-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-3-(trifluoromethyl)-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851048-82-3 CAPLUS

CN 2(1H)-Pyridinone, 1-[[4-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]methyl]-5-(trifluoromethyl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851048-84-5 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-[(4,6-dimethyl-2-pyrimidinyl)methylamino]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851048-85-6 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl)(4'-fluoro[1,1'-biphenyl]-4-yl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851048-86-7 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)(3'-fluoro[1,1'-biphenyl]-4-yl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851048-87-8 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl) [4-(2-pyridinyl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851048-88-9 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(3-pyridinyl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851048-89-0 CAPLUS

CN Benzonitrile, 4-[4-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenoxy]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851048-90-3 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(phenoxymethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851048-91-4 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(3,5-dimethyl-4-isoxazolyl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

RN 851048-93-6 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(5-oxazolyl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

RN 851048-94-7 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl)[4-(2-ethyl-2H-tetrazol-5-yl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851048-95-8 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(1H-pyrrol-1-yl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851048-96-9 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(3,5-dimethyl-1H-pyrazol-1-yl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851048-97-0 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

•x HCl

RN 851048-98-1 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(4-morpholinyl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851049-00-8 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[3-(phenylmethoxy)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851049-01-9 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl) [3-(3-pyridinylmethoxy)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851049-02-0 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[3-(2-pyrazinylmethoxy)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851049-03-1 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[3-(5-methyl-1H-tetrazol-1-yl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851049-04-2 CAPLUS

CN 2-Pyrrolidinone, 1-[3-[(4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl)carbonyl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851049-05-3 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851049-06-4 CAPLUS

CN 4-Pyridinecarboxamide, N-[3-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851049-07-5 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl)[3-(3-pyridinyl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

•x HCl

RN 851049-08-6 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4'-(2-oxazolyl)[1,1'-biphenyl]-4-yl]-, hydrochloride (1:?) (CA INDEX NAME)

$$C - N$$

•x HCl

RN 851049-09-7 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl)[4'-(2-methyl-4-oxazolyl)[1,1'-biphenyl]-4-yl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851049-10-0 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl)[4'-(2-methyl-5-oxazolyl)[1,1'-biphenyl]-4-yl]-, hydrochloride (1:?) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

●x HCl

RN 851049-11-1 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-y1)[4'-(5-methyl-1,2,4-oxadiazol-3-y1)[1,1'-biphenyl]-4-y1]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851049-12-2 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(2-oxazolyl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851049-19-9 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \hline \\ N-O \end{array}$$

•x HCl

RN 851048-52-7 CAPLUS

CN Methanone, (4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]- (CA INDEX NAME)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD

(4 CITINGS)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:238692 CAPLUS

DOCUMENT NUMBER: 142:316849

TITLE: Preparation of phthalazinones as PARP inhibitors INVENTOR(S): Martin, Niall Morrison Barr; Smith, Graeme Cameron;

Jackson, Stephen Philip; Loh, Vincent M., Jr.; Cockcroft, Xiao-Ling Fan; Matthews, Ian Timothy Williams; Menear, Keith Allan; Kerrigan, Frank;

Ashworth, Alan

PATENT ASSIGNEE(S): Kudos Pharmaceuticals Limited, UK; Maybridge Limited

SOURCE:

U.S. Pat. Appl. Publ., 67 pp., Cont.-in-part of U.S.

Ser. No. 799,154.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | API | PLICATION NO. | | DATE | |
|-----------------------------|---------|----------------------|----------|----------------------------|----------|----------|--|
| US 20050059663 | A1 | 20050317 | US | 2004-876080 | _ | 20040624 | |
| US 7449464 ZA 2005007097 | B2 | 20081111 20060628 | 17.7\ | 2005-7097 | | 20050905 | |
| US 20060149059 | A A1 | 20060628 | US | 2005-7097 | | 20050905 | |
| ZA 200600149009 | A | 20071227 | ZA | | | 20051223 | |
| JP 2008001718 | A | 20080110 | | 2007-226723 | | 20070831 | |
| JP 4268651 | В2 | 20090527 | | | | | |
| US 20080200469 | A1 | 20080821 | US | 2008-109260 | | 20080424 | |
| JP 2009079056 | A | 20090416 | JP | 2008-260806 | | 20081007 | |
| PRIORITY APPLN. INFO.: | | | GB | | А | 20030312 | |
| | | | US | 2003-454995P | Ρ | 20030314 | |
| | | | US | 2003-493399P | P | 20030806 | |
| | | | US | 2003-526244P | P | 20031201 | |
| | | | US | 2004-799154 | A2 | 20040312 | |
| | | | JP | 2006-505955 2004-876080 | A3 A3 | 20040312 | |
| | | | US JP | 2004-876080 | | 20040624 | |
| | | 410 0460 | | 2007 220725 | 45 | 200,0001 | |

OTHER SOURCE(S): CASREACT 142:316849; MARPAT 142:316849

GΙ

RN

The title compds. [I; A and B together represent (un)substituted fused aromatic ring; X = NRx or CRxRy; if X= NRx then n = 1 or 2 and if X = CRxRy then n = 1; Rx = H, (un)substituted C1-20 alkyl, C5-20 aryl, C3-20 heterocyclyl, amido, thioamido, ester, acyl, and sulfonyl groups; Ry = H, OH, NH2; or Rx and Ry may together form a spiro(C3-7)cycloalkyl or heterocyclyl group; R11 and R12 are both H, or when X = CRxRy, R11, R12, Rx and Ry, together with the carbon atoms to which they are attached, may form (un)substituted fused aromatic ring; R1 = H, halo], were prepared Thus, reacting 3-(4-oxo-3,4-dihydrophthalazin-1-ylmethyl)benzoic acid (preparation given) with tert-Bu 1-piperazinecarboxylate afforded 77% II which had IC50 of < 0.02 μ M against PARP. All compds. I tested had a IC50 of < 0.1 μ M in the PARP assay. The pharmaceutical composition comprising the compound I is claimed.

IT 848136-26-5P 848136-28-7P 848136-48-1P 848136-50-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phthalazinones as PARP inhibitors for use in the treatment of cancer which is deficient in HR dependent DNA DSB repair pathway) 848136-26-5 CAPLUS

CN 1(2H)-Phthalazinone, 4-[[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-4-fluorophenyl]methyl]- (CA INDEX NAME)

RN 848136-28-7 CAPLUS

CN 1(2H)-Phthalazinone, 4-[[3-[[4-(cyclohexylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-4-fluorophenyl]methyl]- (CA INDEX NAME)

RN 848136-48-1 CAPLUS

CN 1(2H)-Phthalazinone, 4-[[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]methyl]- (CA INDEX NAME)

RN 848136-50-5 CAPLUS

CN 1(2H)-Phthalazinone, 4-[[3-[[4-(cyclohexylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]methyl]- (CA INDEX NAME)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD

(4 CITINGS)

REFERENCE COUNT: 261 THERE ARE 261 CITED REFERENCES AVAILABLE FOR

THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L16 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

2004:718640 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 141:243574

TITLE: Preparation of substituted naphthalenesulfonamides as

CCR8 antagonists

Jin, Jian; Kerns, Jeffrey K.; Shi, Dongchuan; Wang, INVENTOR(S):

Feng; Wang, Yonghui

SmithKline Beecham Corporation, USA PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATI | PATENT NO. | | | | KIND DATE | | | APPLICATION NO. | | | | | | | DATE | | | |
|--|--------------------------|--|--|--|--|--|--|--|--|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|--------------------------------|--|
| | 2004074438 2004074438 | | | A2 2004090 A3 2005022 | | | | | | | | | 20040213 | | | | | |
| | | CN, GE, LK, BW, BG, MC, | CO, GH, LR, GH, CH, NL, | CR, GM, LS, GM, CY, PT, | CU, HR, LT, KE, CZ, RO, | CZ, HU, LU, LS, DE, SE, | AU, DE, ID, LV, MW, DK, SI, SN, | DK, IL, MA, MZ, EE, SK, | DM, IN, MD, SD, ES, TR, | DZ, IS, MG, SL, FI, | EC, JP, MK, SZ, FR, | EE, KE, MN, TZ, GB, | EG, KG, MW, UG, GR, | ES, KP, MX, ZM, HU, | FI, KR, MZ, ZW, IE, | GB, KZ, NA, AT, IT, | GD, LC, NI BE, LU, | |
| PRIORITY APPLN. INFO.: OTHER SOURCE(S): GI | | | | | MAR: | PAT | 141: | 2435 | | US 2 | 003- | 4474 | 50P | 1 | P 2 | 0030: | 214 | |

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

The title compds. [I; n = 0-6; m = 1-4; p = 1-4; Ar = (un) substituted AΒ 2-naphthyl, benzo[1,3]dioxolyl, quinolinyl, etc.; R1, R6 = H, alkyl,

cycloalkylalkyl, phenylalkyl; R2-R5=H, alkyl, alkoxy, halo, etc.; R7=H, alkyl, cycloalkylalkyl, phenylalkyl], useful for inhibiting the chemokine receptor nominated CCR8 (no data given), were prepared E.g., a multi-step synthesis of the sulfonamide II, starting from Et 3-aminobenzoate and using DMHB resin as solid support, was given. The pharmaceutical composition comprising the compound I is claimed.

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted naphthalenesulfonamides as CCR8 antagonists for treating respiratory condition)

RN 749866-39-5 CAPLUS

CN 2-Naphthalenesulfonamide, N-[3-[[4-(cyclohexylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 749866-38-4 CMF C29 H35 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 749866-43-1 CAPLUS

CN 2-Naphthalenesulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749866-86-2 CAPLUS

CN 2-Naphthalenesulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-4-methoxyphenyl]- (CA INDEX NAME)

RN 749866-87-3 CAPLUS

CN 2-Naphthalenesulfonamide, N-[5-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-2-methoxyphenyl]- (CA INDEX NAME)

RN 749866-88-4 CAPLUS

CN 2-Naphthalenesulfonamide, N-[5-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-2-methylphenyl]- (CA INDEX NAME)

RN 749866-89-5 CAPLUS

CN 2-Naphthalenesulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-2-methylphenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ S - NH & C - N & N - CH_2 \end{array}$$

RN 749866-90-8 CAPLUS

CN 2-Naphthalenesulfonamide, N-[4-chloro-3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749866-91-9 CAPLUS

CN 2-Naphthalenesulfonamide, N-[4-bromo-3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749866-92-0 CAPLUS

CN 2-Naphthalenesulfonamide, N-[2-chloro-5-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749866-93-1 CAPLUS

CN 2-Naphthalenesulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-5-nitrophenyl]- (CA INDEX NAME)

RN 749866-99-7 CAPLUS

CN 1,3-Benzodioxole-5-sulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749867-00-3 CAPLUS

CN 1,3-Benzodioxole-5-sulfonamide, N-[5-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-2-methylphenyl]- (CA INDEX NAME)

RN 749867-05-8 CAPLUS

CN 1,4-Benzodioxin-6-sulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-2,3-dihydro- (CA INDEX NAME)

RN 749867-07-0 CAPLUS

CN 1,4-Benzodioxin-6-sulfonamide, N-[5-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-2-methylphenyl]-2,3-dihydro- (CA INDEX NAME)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Page 87

L16 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:718298 CAPLUS

DOCUMENT NUMBER: 141:243573

TITLE: Preparation of substituted benzenesulfonamides as CCR8

antagonists

INVENTOR(S): Jin, Jian; Kerns, Jeffrey K.; Wang, Feng; Wang,

Yonghui

PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 32 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PAT | PATENT NO. | | | | | D | DATE | | | APPLICATION NO. | | | | | DATE | | | |
|----------------------|------------|--|---------------------------------|---------------------------------|--|---------------------------------|--|--|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|--------------------------------|--|
| | | | | | | | 20040902 | | WO 2004-US4256 | | | | 20040213 | | | | | |
| WO | ₩: | AE, CN, GE, LK, BW, BG, | AG, CO, GH, LR, GH, | CR, GM, LS, GM, CY, | AM, CU, HR, LT, KE, CZ, | AT, CZ, HU, LU, DE, | AU, DE, ID, LV, MW, DK, | AZ, DK, IL, MA, MZ, EE, | DM, IN, MD, SD, ES, | DZ, IS, MG, SL, FI, | EC, JP, MK, SZ, FR, | EE, KE, MN, TZ, GB, | EG, KG, MW, UG, GR, | ES, KP, MX, ZM, HU, | FI, KR, MZ, ZW, IE, | GB, KZ, NA, AT, IT, | GD, LC, NI BE, LU, | |
| PRIORITY OTHER SO | | GQ, LN. | GW, INFO | ML, | MR, | NE, | SI, SN, 141: | TD, | TG | BF, US 2 | , | , | ŕ | ŕ | , | GA, | , | |

AB The title compds. [I; n = 0-6; m = 1-4; p = 1-4; Ar = (un) substituted Ph, thienyl, furanyl, pyridinyl; R1, R6 = H, alkyl, cycloalkylalkyl,

GI

phenylalkyl; R2-R5 = H, alkyl, alkoxy, halo, etc.; R7 = H, alkyl, cycloalkylalkyl, phenylalkyl], useful for inhibiting the chemokine receptor nominated CCR8 (no data given), were prepared E.g., a multi-step synthesis of the sulfonamide II, starting from Me 3-aminobenzoate and using DMHB resin as solid support, was given. The pharmaceutical composition comprising the compound I is claimed.

749881-98-9P ΙT 749881-87-6P 749881-88-7P 749882-32-4P 749882-38-0P 749882-42-6P 749882-46-0P 749882-58-4P 749882-72-2P 749882-90-4P 749883-14-5P 749883-16-7P 749883-36-1P 749883-51-0P 749883-62-3P 749883-63-4P 749883-71-4P 749883-94-1P 749884-33-1P 749884-34-2P 749884-35-3P 749884-36-4P 749884-37-5P 749884-38-6P 749884-39-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted benzenesulfonamides as CCR8 antagonists for treating respiratory condition)

RN 749881-87-6 CAPLUS

CN Benzenesulfonamide, 3-chloro-N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749881-88-7 CAPLUS

CN Benzenesulfonamide, 3-chloro-N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 749881-87-6 CMF C22 H26 C1 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 749881-98-9 CAPLUS

CN Benzenesulfonamide, 3,4-dichloro-N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749882-32-4 CAPLUS

CN Benzenesulfonamide, 3-chloro-N-[3-[[4-(cyclohexylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749882-38-0 CAPLUS

CN Benzenesulfonamide, 2,4,5-trichloro-N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749882-42-6 CAPLUS

CN Benzenesulfonamide, 2,4,5-trichloro-N-[3-[[4-(cyclohexylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749882-46-0 CAPLUS

CN Benzenesulfonamide, 2,4-dichloro-N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749882-58-4 CAPLUS

CN Benzenesulfonamide, 3,4-dibromo-N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749882-72-2 CAPLUS

CN Benzenesulfonamide, 3-bromo-N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749882-90-4 CAPLUS

CN Benzenesulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-4-methoxy- (CA INDEX NAME)

RN 749883-14-5 CAPLUS

CN Benzenesulfonamide, N-[3-[[4-(cyclohexylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-3,4-dimethoxy- (CA INDEX NAME)

RN 749883-16-7 CAPLUS

CN Benzenesulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-3,4-dimethoxy- (CA INDEX NAME)

RN 749883-36-1 CAPLUS

CN [1,1'-Biphenyl]-4-sulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749883-51-0 CAPLUS

CN 3-Thiophenesulfonamide, 2,5-dichloro-N-[3-[[4-(cyclohexylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749883-62-3 CAPLUS

CN Benzenesulfonamide, 4-chloro-N-[3-[[4-(cyclohexylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-2,5-dimethyl- (CA INDEX NAME)

RN 749883-63-4 CAPLUS

CN Benzenesulfonamide, 4-chloro-N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-2,5-dimethyl- (CA INDEX NAME)

RN 749883-71-4 CAPLUS

CN Benzenesulfonamide, 5-bromo-N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-2-methoxy- (CA INDEX NAME)

RN 749883-94-1 CAPLUS

CN 2-Thiophenesulfonamide, 4,5-dibromo-N-[3-[[4-(cyclopropylmethyl)hexahydro-

1H-1, 4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

RN 749884-33-1 CAPLUS

CN Benzenesulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-4-methoxyphenyl]-3,4-dimethoxy- (CA INDEX NAME)

RN 749884-34-2 CAPLUS

CN Benzenesulfonamide, N-[5-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-2-methoxyphenyl]-3,4-dimethoxy- (CA INDEX NAME)

RN 749884-35-3 CAPLUS

CN Benzenesulfonamide, N-[5-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-2-methylphenyl]-3,4-dimethoxy- (CA INDEX NAME)

RN 749884-36-4 CAPLUS

CN Benzenesulfonamide, N-[3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]-2-methylphenyl]-3,4-dimethoxy- (CA INDEX NAME)

RN 749884-37-5 CAPLUS

CN Benzenesulfonamide, N-[4-chloro-3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-3,4-dimethoxy- (CA INDEX NAME)

RN 749884-38-6 CAPLUS

CN Benzenesulfonamide, N-[4-bromo-3-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-3,4-dimethoxy- (CA INDEX NAME)

RN 749884-39-7 CAPLUS

CN Benzenesulfonamide, N-[2-chloro-5-[[4-(cyclopropylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]-3,4-dimethoxy- (CA INDEX NAME)

4

OS.CITING REF COUNT:

THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD

(4 CITINGS)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:777909 CAPLUS

DOCUMENT NUMBER: 137:295253

TITLE: Method for preparing monocyclic N-acyl aminolactam

compounds and their combinatorial libraries

INVENTOR(S): Cheng, Jie Fei; Chen, Mi; Nadzan, Alex PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| P | PATENT NO. | | | | KIND DATE | | | APPLICATION NO. | | | | | | DATE | | | |
|--------|---------------|------|--------|-----|-----------|-----|------|-----------------|------|------|-------|----------|-----|------|-----|------|-----|
| w | 0 2002 | 0791 | 72 | | A1 | | 2002 | 1010 | | WO 2 | 001- | US51 | 579 | | 2 | 0011 | 210 |
| | W: | ΑE, | AG, | AL, | AM, | AT, | ΑU, | ΑZ, | BA, | BB, | BG, | BR, | BY, | BZ, | CA, | CH, | CN, |
| | | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DΖ, | EC, | EE, | ES, | FI, | GB, | GD, | GE, | GH, |
| | | GM, | HR, | ΗU, | ID, | IL, | IN, | IS, | JP, | ΚE, | KG, | ΚP, | KR, | ΚZ, | LC, | LK, | LR, |
| | | LS, | LT, | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | ΜZ, | NO, | NZ, | PH, | PL, |
| | | PT, | RO, | RU, | SD, | SE, | SG, | SI, | SK, | SL, | ТJ, | TM, | TR, | TT, | TZ, | UA, | UG, |
| | | US, | UΖ, | VN, | YU, | ZA, | ZW | | | | | | | | | | |
| | RW: | GH, | GM, | ΚE, | LS, | MW, | ΜZ, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AT, | BE, | CH, |
| | | CY, | DE, | DK, | ES, | FI, | FR, | GB, | GR, | ΙE, | ΙΤ, | LU, | MC, | NL, | PT, | SE, | TR, |
| | | BF, | ВJ, | CF, | CG, | CI, | CM, | GΑ, | GN, | GQ, | GW, | ML, | MR, | ΝE, | SN, | TD, | ΤG |
| A | AU 2001297757 | | | A1 | 20021015 | | | | AU 2 | 001- | 2977. | 20011210 | | | | | |
| PRIORI | TY APP | LN. | INFO | .: | | | | | | US 2 | 000- | 2550 | 92P | | P 2 | 0001 | 212 |
| | | | | | | | | | | WO 2 | 001- | US51. | 579 | 1 | W 2 | 0011 | 210 |

OTHER SOURCE(S): MARPAT 137:295253

GΙ

AB Piperazin-2-ones, perhydro-1, 4-diazepin-2(or 5)-ones, and 1,5-diazocan-2-ones I [R1, R6 = alkyl, aryl, heterocyclyl, heteroaryl; R2, R3, R5 = H or any group given for R1; X = CH2 or CH2CH2; Z = CHR4 or R9CHCHR8, where R4, R8, R9 = any group given for R2] were prepared via four-component reaction of a polymer bound isocyanide R1NC, a ketone R2COR3 or aldehyde R2CHO, a protected amino acid P-Z-CO2H (P = protecting group), and a protected α- or β-amino acetal, deprotection of the polymer-bound acetal, reaction of the polymer-bound aldehyde with an acid R5CO2H and an isocyanide R6NC, and cleavage from the resin. The method was applied to the preparation of 22 title compds., including piperazin-2-ones I [X = CH2; Z = CHR4; R1 = (CH2)5CO2H; R2 = PhCH2CH2, i-Pr, cyclohexyl; R3 = H; R4 = Me, i-Pr, H; R5 = PhCH2CH2, C6H4NO2-3, C6H4CO2Me-4; R6 = Bu, t-Bu, PhCH2].

IT 467469-38-1P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of monocyclic N-acyl aminolactam compds. by solid-phase four-component reaction)

RN 467469-38-1 CAPLUS

CN Benzoic acid, 4-[[4-[2-[(5-carboxypentyl)amino]-1-cyclohexyl-2-oxoethyl]-7[[[(diethoxyphosphinyl)methyl]amino]carbonyl]hexahydro-3-oxo-1H-1,4diazepin-1-yl]carbonyl]-, 1-methyl ester (CA INDEX NAME)

REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:761511 CAPLUS

DOCUMENT NUMBER: 123:169669

ORIGINAL REFERENCE NO.: 123:30303a,30306a

TITLE: Preparation of diazepinoquinolonecarboxylates as

antibacterial agents

INVENTOR(S): Perrin, Claude

PATENT ASSIGNEE(S): Bouchara SA, Fr.

SOURCE: Fr. Demande, 30 pp.

CODEN: FRXXBL

Ι

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|----------|
| | | | | |
| FR 2706459 | A1 | 19941223 | FR 1993-7293 | 19930617 |
| FR 2706459 | B1 | 19950804 | | |
| PRIORITY APPLN. INFO.: | | | FR 1993-7293 | 19930617 |
| OTHER SOURCE(S): | MARPAT | 123:169669 | | |
| GI | | | | |

AB Title compds. (I; R = H, alkyl, alkanoyl, alkoxycarbonyl, arylsulfonyl, etc.; R1 = halo, alkoxy) were prepared Thus, 1-cyclopropyl-6,7,8-trifluoro-4-quinolone-3-carboxylic acid was condensed with homopiperazine to give I (R = H, R1 = F). Data for antibacterial activity of selected title compds. were given.

IT 167018-78-2P 167018-80-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diazepinoquinolonecarboxylates as antibacterial agents) RN 167018-78-2 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-7-[hexahydro-4-(2-sulfobenzoyl)-1H-1,4-diazepin-1-yl]-1,4-dihydro-4-oxo- (CA INDEX NAME)

RN 167018-80-6 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6-fluoro-7-[hexahydro-4-(2-sulfobenzoyl)-1H-1,4-diazepin-1-yl]-1,4-dihydro-4-oxo- (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 381 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439236-84-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclobutanecarboxamide, N-[2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C28 H34 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 375 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439236-98-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopentanecarboxamide, N-[2-(4-benzoylhexahydro-1H-1,4-diazepin-1-

yl)-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C29 H37 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 376 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439236-96-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopentanecarboxamide, N-[2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C29 H36 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 377 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439236-92-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopentanecarboxamide, N-[2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C29 H36 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 378 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439236-90-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclobutanecarboxamide, N-[2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C30 H39 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 379 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439236-88-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclobutanecarboxamide, N-[2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C29 H34 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 380 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

439236-86-9 REGISTRY RN

ED Entered STN: 18 Jul 2002

Cyclobutanecarboxamide, N-[2-[4-[4-(1,1-CN dimethylethyl)benzoyl]hexahydro-1H-1,4-diazepin-1-yl]-5-(1piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MFC32 H43 N5 O3

Chemical Library SR

Supplier: Ambinter

L18 ANSWER 365 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-20-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C28 H32 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 366 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-18-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-[4-(1,1-dimethylethyl)benzoyl]hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C31 H41 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 367 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-14-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C27 H33 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 368 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-12-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C27 H32 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 369 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-09-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopentanecarboxamide, N-[2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C29 H36 C1 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 370 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-08-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C27 H32 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 371 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-07-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopentanecarboxamide, N-[2-[4-(3,5-difluorobenzoy1)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C29 H35 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 372 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-05-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopentanecarboxamide, N-[2-[4-(3,4-dimethoxybenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-5-(1-piperazinylcarbony1)pheny1]- (CA INDEX NAME)

MF C31 H41 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 373 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-04-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopentanecarboxamide, N-[2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C30 H36 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 374 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-02-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopentanecarboxamide, N-[2-[4-[4-(1,1-dimethylethyl)benzoyl]hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C33 H45 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 355 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-44-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C30 H37 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 356 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-42-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(3,4-dimethoxybenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-5-(1-piperazinylcarbony1)pheny1]- (CA INDEX NAME)

MF C32 H43 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 357 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-40-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C31 H38 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 358 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-38-4 REGISTRY

ED Entered STN: 18 Jul 2002

Cyclohexanecarboxamide, N-[2-[4-[4-(1,1-CN dimethylethyl)benzoyl]hexahydro-1H-1,4-diazepin-1-yl]-5-(1piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MFC34 H47 N5 O3

Chemical Library SR

Supplier: Ambinter

L18 ANSWER 359 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-34-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C30 H39 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 360 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-32-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C30 H38 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 361 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-28-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C30 H38 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 362 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-26-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C27 H32 C1 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 363 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-24-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(3,5-difluorobenzoy1)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C27 H31 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 364 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439237-22-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(3,4-dimethoxybenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C29 H37 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 345 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439243-77-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(4-fluorobenzoyl)amino]- (CA INDEX NAME)

MF C32 H36 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 346 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439243-75-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-fluorobenzoyl)amino]-4-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C32 H35 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 347 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439243-73-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-fluorobenzoyl)amino]-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C32 H35 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 348 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439240-20-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclobutanecarboxamide, N-[2-[4-(3,5-difluorobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-5-[(hexahydro-1H-1,4-diazepin-1-y1)carbony1]pheny1]- (CA INDEX NAME)

MF C29 H35 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

PAGE 1-A

PAGE 2-A

L18 ANSWER 349 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439240-19-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclobutanecarboxamide, N-[2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]- (CA INDEX NAME)

MF C31 H41 N5 O5

SR Chemical Library

Supplier: Ambinter

PAGE 1-A

PAGE 2-A

L18 ANSWER 350 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439240-18-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclobutanecarboxamide, N-[2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-(CA INDEX NAME)

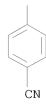
MF C30 H36 N6 O3

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RN 439240-16-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclobutanecarboxamide, N-[2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]- (CA INDEX NAME)

MF C29 H37 N5 O3

SR Chemical Library

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L18 ANSWER 352 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439240-15-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclobutanecarboxamide, N-[2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-(CA INDEX NAME)

MF C29 H36 F N5 O3

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RN 439240-13-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclobutanecarboxamide, N-[2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-(CA INDEX NAME)

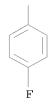
MF C29 H36 F N5 O3

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RN 439237-46-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C30 H38 C1 N5 O3

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C1 C N NH C O NH

L18 ANSWER 335 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439243-99-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(3-fluorobenzoyl)amino]-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C32 H35 F2 N5 O3

SR Chemical Library

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RN 439243-97-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide,
N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C33 H35 F2 N5 O5

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RN 439243-95-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

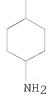
MF C34 H39 N5 O6

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RN 439243-92-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide,
N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

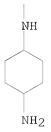
MF C35 H41 N5 O7

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L18 ANSWER 339 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439243-90-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

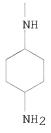
MF C34 H36 N6 O5

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RN 439243-88-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)phenyl]- (CA INDEX NAME)

MF C33 H37 N5 O5

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NH2

L18 ANSWER 341 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439243-86-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

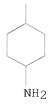
MF C33 H36 F N5 O5

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RN 439243-83-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C33 H36 F N5 O5

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L18 ANSWER 343 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439243-81-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-fluorobenzoyl)amino]-4[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C33 H38 F N5 O4

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L18 ANSWER 344 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439243-79-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(4-fluorobenzoyl)amino]- (CA INDEX NAME)

MF C34 H40 F N5 O5

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L18 ANSWER 325 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-12-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(4-nitrobenzoyl)amino]- (CA INDEX NAME)

MF C32 H35 F N6 O5

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L18 ANSWER 326 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-10-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(4-nitrobenzoyl)amino]- (CA INDEX NAME)

MF C32 H35 F N6 O5

SR Chemical Library

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L18 ANSWER 327 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-09-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-(benzoylamino)-4-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C33 H39 N5 O4

SR Chemical Library

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L18 ANSWER 328 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-08-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-(benzoylamino)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C34 H41 N5 O5

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L18 ANSWER 329 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-07-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-(benzoylamino)-4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C33 H36 N6 O3

SR Chemical Library

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L18 ANSWER 330 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-06-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-(benzoylamino)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

MF C32 H37 N5 O3

SR Chemical Library

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RN 439244-05-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-(benzoylamino)-4-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C32 H36 F N5 O3

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RN 439244-03-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-(benzoylamino)-4-[4-(4fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C32 H36 F N5 O3

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RN 439244-02-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-fluorobenzoyl)amino]- (CA INDEX NAME)

MF C34 H40 F N5 O5

SR Chemical Library

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L18 ANSWER 334 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-01-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(3-fluorobenzoyl)amino]- (CA INDEX NAME)

MF C32 H36 F N5 O3

SR Chemical Library

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L18 ANSWER 315 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-26-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, 3-(acetylamino)-N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-

methoxybenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C28 H37 N5 O4

SR Chemical Library

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L18 ANSWER 316 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-23-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, 3-(acetylamino)-N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)- (CA INDEX NAME)

MF C27 H35 N5 O3

SR Chemical Library

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L18 ANSWER 317 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-22-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, 3-(acetylamino)-N-(4-aminocyclohexyl)-4-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C27 H34 F N5 O3

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C NH C NH2

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RN 439244-21-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[[4-(1,1-dimethylethyl)benzoyl]amino]- (CA INDEX NAME)

MF C36 H43 F2 N5 O3

SR Chemical Library

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L18 ANSWER 319 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-20-9 REGISTRY

ED Entered STN: 18 Jul 2002

Benzamide, N-(4-aminocyclohexyl)-3-[[4-(1,1-CN dimethylethyl)benzoyl]amino]-4-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4diazepin-1-yl]- (CA INDEX NAME)

C37 H47 N5 O4 MF

Chemical Library SR

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L18 ANSWER 320 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-18-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[[4-(1,1-dimethylethyl)benzoyl]amino]- (CA INDEX NAME)

MF C38 H49 N5 O5

SR Chemical Library

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L18 ANSWER 321 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-17-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[[4-(1,1-dimethylethyl)benzoyl]amino]- (CA INDEX NAME)

MF C37 H44 N6 O3

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RN 439244-16-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[[4-(1,1-dimethylethyl)benzoyl]amino]- (CA INDEX NAME)

MF C36 H45 N5 O3

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L18 ANSWER 323 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-15-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[[4-(1,1-dimethylethyl)benzoyl]amino]-4-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C36 H44 F N5 O3

SR Chemical Library

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L18 ANSWER 324 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-13-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[[4-(1,1-dimethylethyl)benzoyl]amino]-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C36 H44 F N5 O3

SR Chemical Library

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L18 ANSWER 305 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-39-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)phenyl]-3,4-dimethoxy- (CA INDEX NAME)

MF C34 H41 N5 O5

SR Chemical Library

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L18 ANSWER 306 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-38-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-dimethoxy-(CA INDEX NAME)

MF C34 H40 F N5 O5

SR Chemical Library

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L18 ANSWER 307 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-36-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-dimethoxy-(CA INDEX NAME)

MF C34 H40 F N5 O5

SR Chemical Library

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L18 ANSWER 308 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-35-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-cyanobenzoyl)amino]-4-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C33 H34 F2 N6 O3

SR Chemical Library

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L18 ANSWER 309 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-34-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-cyanobenzoyl)amino]-4[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C34 H38 N6 O4

SR Chemical Library

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L18 ANSWER 310 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-32-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-cyanobenzoyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C35 H40 N6 O5

SR Chemical Library

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L18 ANSWER 311 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-31-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-cyanobenzoyl)amino]-4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C34 H35 N7 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 312 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-30-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(4-cyanobenzoyl)amino]- (CA INDEX NAME)

MF C33 H36 N6 O3

SR Chemical Library

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L18 ANSWER 313 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-29-8 REGISTRY

ED Entered STN: 18 Jul 2002

Benzamide, N-(4-aminocyclohexyl)-3-[(4-cyanobenzoyl)amino]-4-[4-(3-CN fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

C33 H35 F N6 O3 MF

Chemical Library SR

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L18 ANSWER 314 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-27-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-cyanobenzoyl)amino]-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C33 H35 F N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 295 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-51-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methoxybenzoyl)amino]- (CA INDEX NAME)

MF C33 H37 F2 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 296 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-50-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]-3-[(3-methoxybenzoyl)amino]- (CA INDEX NAME)

MF C34 H41 N5 O5

SR Chemical Library

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L18 ANSWER 297 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-49-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methoxybenzoyl)amino]- (CA INDEX NAME)

MF C35 H43 N5 O6

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 298 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-48-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methoxybenzoyl)amino]- (CA INDEX NAME)

MF C34 H38 N6 O4

SR Chemical Library

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L18 ANSWER 299 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-47-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methoxybenzoyl)amino]- (CA INDEX NAME)

MF C33 H38 F N5 O4

SR Chemical Library

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L18 ANSWER 300 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-45-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methoxybenzoyl)amino]- (CA INDEX NAME)

MF C33 H38 F N5 O4

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L18 ANSWER 301 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-44-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-dimethoxy-(CA INDEX NAME)

MF C34 H39 F2 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 302 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-43-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-3,4-dimethoxy- (CA INDEX NAME)

MF C35 H43 N5 O6

SR Chemical Library

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L18 ANSWER 303 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-41-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-dimethoxy-(CA INDEX NAME)

MF C36 H45 N5 O7

SR Chemical Library

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L18 ANSWER 304 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-40-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-dimethoxy-(CA INDEX NAME)

MF C35 H40 N6 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 285 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-66-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C35 H43 N5 O5

SR Chemical Library

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L18 ANSWER 286 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-65-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C34 H38 N6 O3

SR Chemical Library

Supplier: Ambinter

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RN 439244-64-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)phenyl]- (CA INDEX NAME)

MF C33 H39 N5 O3

SR Chemical Library

Supplier: Ambinter

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-C-NH-} & & \\ & & \\ & &$$

L18 ANSWER 288 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-63-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C33 H38 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 289 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-61-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[[3-(trifluoromethyl)benzoyl]amino]- (CA INDEX NAME)

MF C33 H34 F5 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 290 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-60-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]-3-[[3-(trifluoromethyl)benzoyl]amino]- (CA INDEX NAME)

MF C34 H38 F3 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 291 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-58-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[[3-(trifluoromethyl)benzoyl]amino]- (CA INDEX NAME)

MF C35 H40 F3 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 292 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-56-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[[3-(trifluoromethyl)benzoyl]amino]- (CA INDEX NAME)

MF C33 H36 F3 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 293 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-54-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-fluorobenzoyl)hexahydro-1H1,4-diazepin-1-yl]-3-[[3-(trifluoromethyl)benzoyl]amino]- (CA INDEX NAME)

MF C33 H35 F4 N5 O3

SR Chemical Library

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L18 ANSWER 294 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-52-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-fluorobenzoyl)hexahydro-1H1,4-diazepin-1-yl]-3-[[3-(trifluoromethyl)benzoyl]amino]- (CA INDEX NAME)

MF C33 H35 F4 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 275 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-80-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)phenyl]-4-methoxy- (CA INDEX NAME)

MF C34 H41 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 276 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-79-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]]-2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-4-methoxy- (CA INDEX NAME)

MF C34 H40 F N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 277 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-77-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]]-2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-4-methoxy- (CA INDEX NAME)

MF C34 H40 F N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 278 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-76-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C32 H35 N7 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 279 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-74-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C31 H35 F N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 280 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-72-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C31 H35 F N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 281 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-71-0 REGISTRY

ED Entered STN: 18 Jul 2002

 $\texttt{CN} \qquad 4-\texttt{Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino]carbonyl]-2-(4-aminocyclohexyl)amino[aminocyclohexyl]-2-(4-aminocyclohexyl)amino$

benzoylhexahydro-1H-1,4-diazepin-1-yl)phenyl]- (CA INDEX NAME)

MF C31 H36 N6 O3

SR Chemical Library

Supplier: Ambinter

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RN 439244-70-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN 4-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C31 H35 F N6 O3

SR Chemical Library

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L18 ANSWER 283 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-69-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C33 H37 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 284 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-68-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]phenyl]- (CA
INDEX NAME)

MF C34 H41 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 265 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-93-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,2,3-Thiadiazole-5-carboxamide,
N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-4-methyl- (CA INDEX NAME)

MF C29 H33 F2 N7 O3 S

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 266 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-92-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,2,3-Thiadiazole-5-carboxamide,
N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-4-methyl- (CA INDEX NAME)

MF C30 H37 N7 O4 S

SR Chemical Library
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RN 439244-91-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,2,3-Thiadiazole-5-carboxamide,
N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-4-methyl-(CA INDEX NAME)

MF C31 H39 N7 O5 S

SR Chemical Library
Supplier: Ambinter

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L18 ANSWER 268 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-90-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,2,3-Thiadiazole-5-carboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-4-methyl- (CA INDEX NAME)

MF C29 H34 F N7 O3 S

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 269 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-89-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

MF C33 H37 F2 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 270 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-88-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

MF C33 H39 N5 O4

SR Chemical Library

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L18 ANSWER 271 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-87-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

MF C33 H38 F N5 O4

SR Chemical Library

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L18 ANSWER 272 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-85-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-4-methoxy(CA INDEX NAME)

MF C35 H43 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 273 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-83-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-4-methoxy-(CA INDEX NAME)

MF C36 H45 N5 O6

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 274 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-82-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-4-methoxy- (CA INDEX NAME)

MF C35 H40 N6 O4

SR Chemical Library

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L18 ANSWER 255 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-07-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(3-methylbenzoyl)amino]- (CA INDEX NAME)

MF C33 H39 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 256 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-06-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methylbenzoyl)amino]- (CA INDEX NAME)

MF C33 H38 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 257 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-04-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methylbenzoyl)amino]- (CA INDEX NAME)

MF C33 H38 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 258 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-03-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(cyclopropylcarbonyl)amino]-4-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C30 H39 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 259 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-02-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(cyclopropylcarbonyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C31 H41 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 260 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-00-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C27 H33 F2 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 261 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-99-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C28 H37 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 262 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-97-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)phenyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C27 H35 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 263 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-96-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C27 H34 F N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 264 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439244-94-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C27 H34 F N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 245 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-20-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-3,4-difluoro-(CA INDEX NAME)

MF C33 H37 F2 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 246 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-18-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-difluoro-(CA INDEX NAME)

MF C34 H39 F2 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 247 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-17-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-difluoro-(CA INDEX NAME)

MF C33 H34 F2 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 248 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-16-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)phenyl]-3,4-difluoro- (CA INDEX NAME)

MF C32 H35 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 249 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-15-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-difluoro-(CA INDEX NAME)

MF C32 H34 F3 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 250 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-13-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-difluoro-(CA INDEX NAME)

MF C32 H34 F3 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 251 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-12-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methylbenzoyl)amino]- (CA INDEX NAME)

MF C33 H37 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 252 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-11-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]-3-[(3-methylbenzoyl)amino]- (CA INDEX NAME)

MF C34 H41 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 253 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-09-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methylbenzoyl)amino]- (CA INDEX NAME)

MF C35 H43 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 254 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-08-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methylbenzoyl)amino]- (CA INDEX NAME)

MF C34 H38 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 235 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-50-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C28 H37 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 236 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-45-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C27 H34 C1 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 237 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-44-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C28 H34 F3 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 238 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-39-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

MF C34 H41 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 239 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-34-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

MF C33 H38 C1 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 240 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-33-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Carbamic acid, [5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

MF C34 H38 F3 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 241 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-29-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-4-methoxy(CA INDEX NAME)

MF C35 H43 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 242 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-25-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]]-2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-4-methoxy- (CA INDEX NAME)

MF C34 H40 C1 N5 O4

SR Chemical Library

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RN 439245-24-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]phenyl]-4methoxy- (CA INDEX NAME)

MF C35 H40 F3 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 244 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-21-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-difluoro-(CA INDEX NAME)

MF C32 H33 F4 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 225 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-13-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(3-fluorobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-5-[(hexahydro-1H-1,4-diazepin-1-y1)carbonyl]phenyl]-(CA INDEX NAME)

MF C28 H34 F N5 O3

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 226 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-11-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(4-fluorobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-5-[(hexahydro-1H-1,4-diazepin-1-y1)carbonyl]phenyl]-(CA INDEX NAME)

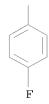
MF C28 H34 F N5 O3

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 227 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-79-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, 3-amino-N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C26 H35 N5 O2

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 228 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-75-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, 3-amino-N-(4-aminocyclohexyl)-4-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C25 H32 C1 N5 O2

SR Chemical Library
Supplier: Ambinter

L18 ANSWER 229 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-73-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-3,4-difluoro-(CA INDEX NAME)

MF C33 H37 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 230 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-67-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-difluoro-(CA INDEX NAME)

MF C32 H34 C1 F2 N5 O3

SR Chemical Library

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L18 ANSWER 231 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-66-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]phenyl]-3,4-difluoro-(CA INDEX NAME)

MF C33 H34 F5 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 232 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-61-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]-3-[(3-methylbenzoyl)amino]- (CA INDEX NAME)

MF C34 H41 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 233 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439245-55-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(3-methylbenzoyl)amino]- (CA INDEX NAME)

MF C33 H38 C1 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 234 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN RN 439245-54-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]-3-[(3-methylbenzoyl)amino]-(CA INDEX NAME)

MF C34 H38 F3 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 215 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-28-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(3,5-difluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]- (CA INDEX NAME)

MF C31 H39 F2 N5 O3

SR Chemical Library

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L18 ANSWER 216 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-26-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]- (CA INDEX NAME)

MF C33 H45 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 217 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-23-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]- (CA INDEX NAME)

MF C31 H41 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 218 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-22-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-(CA INDEX NAME)

MF C31 H40 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 219 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-20-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-(CA INDEX NAME)

MF C31 H40 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 220 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-19-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(3,5-difluorobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-5-[(hexahydro-1H-1,4-diazepin-1-y1)carbonyl]phenyl]-(CA INDEX NAME)

MF C28 H33 F2 N5 O3

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 221 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-18-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]-2-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C29 H37 N5 O4

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 222 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-17-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-(CA INDEX NAME)

MF C30 H39 N5 O5

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 223 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-16-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-(CA INDEX NAME)

MF C29 H34 N6 O3

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 224 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439246-14-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-(4-benzoylhexahydro-1H-1,4-diazepin-1-y1)-5-[(hexahydro-1H-1,4-diazepin-1-y1)carbonyl]phenyl]- (CA INDEX NAME)

MF C28 H35 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 205 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-03-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-(benzoylamino)-4-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C32 H36 C1 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 206 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-00-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(3-fluorobenzoyl)amino]-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C33 H38 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 207 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439247-98-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(3-fluorobenzoyl)amino]-4-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C33 H35 F4 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 208 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439247-94-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C34 H39 N5 O5

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 209 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439247-36-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

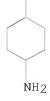
MF C33 H36 C1 N5 O5

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 210 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439247-35-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN 1,3-Benzodioxole-5-carboxamide,
N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

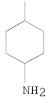
MF C34 H36 F3 N5 O5

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 211 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439247-30-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-fluorobenzoyl)amino]-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C33 H38 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 212 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439247-25-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-fluorobenzoyl)amino]-4[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]- (CA
INDEX NAME)

MF C33 H35 F4 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 213 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439247-17-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C31 H38 F3 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 214 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439247-10-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]-5-(1piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MFC28 H32 F3 N5 O3

Chemical Library SR

Supplier: Ambinter

L18 ANSWER 195 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-32-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(4-cyanobenzoyl)amino]- (CA INDEX NAME)

MF C33 H35 C1 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 196 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-31-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-cyanobenzoyl)amino]-4[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]- (CA
INDEX NAME)

MF C34 H35 F3 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 197 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-29-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, 3-(acetylamino)-N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C28 H37 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 198 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-26-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, 3-(acetylamino)-N-(4-aminocyclohexyl)-4-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C27 H34 C1 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 199 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-21-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[[4-(1,1-dimethylethyl)benzoyl]amino]-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C37 H47 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 200 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-16-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-chlorobenzoyl)hexahydro-1H1,4-diazepin-1-yl]-3-[[4-(1,1-dimethylethyl)benzoyl]amino]- (CA
INDEX NAME)

MF C36 H44 C1 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 201 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-15-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[[4-(1,1-dimethylethyl)benzoyl]amino]-4-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C37 H44 F3 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 202 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-14-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]-3-[(4-nitrobenzoyl)amino]- (CA INDEX NAME)

MF C33 H38 N6 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 203 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-11-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(4-nitrobenzoyl)amino]- (CA INDEX NAME)

MF C32 H35 C1 N6 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 204 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-06-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-(benzoylamino)-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C33 H39 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 185 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-88-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN 4-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C31 H35 C1 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 186 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-87-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN 4-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]phenyl]-(CA INDEX NAME)

MF C32 H35 F3 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 187 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-80-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C34 H41 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 188 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-71-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C33 H38 C1 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 189 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-69-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzeneacetamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]phenyl](CA INDEX NAME)

MF C34 H38 F3 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 190 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-66-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]-3-[[3-(trifluoromethyl)benzoyl]amino]- (CA INDEX NAME)

MF C34 H38 F3 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 191 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-50-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]phenyl]-3,4-dimethoxy- (CA INDEX NAME)

MF C35 H43 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 192 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-43-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]-3,4-dimethoxy-(CA INDEX NAME)

MF C34 H40 C1 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 193 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-42-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]phenyl]-3,4-dimethoxy-(CA INDEX NAME)

MF C35 H40 F3 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 194 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-38-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-3-[(4-cyanobenzoyl)amino]-4[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]- (CA INDEX NAME)

MF C34 H38 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 175 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439252-33-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(cyclopropylcarbonyl)amino]benzoyl]amino]-4-fluoro-(CA INDEX NAME)

MF C33 H32 F N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 176 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439251-59-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(2,4-dichlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]- (CA INDEX NAME)

MF C31 H39 C12 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 177 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439251-49-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclohexanecarboxamide, N-[2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-5-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-(CA INDEX NAME)

MF C31 H40 C1 N5 O3

SR Chemical Library

Supplier: Ambinter

10/576,492

L18 ANSWER 178 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439251-48-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(2,4-dichlorobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-5-[(hexahydro-1H-1,4-diazepin-1-y1)carbonyl]phenyl]-(CA INDEX NAME)

MF C28 H33 C12 N5 O3

SR Chemical Library

Supplier: Ambinter

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10/576,492

L18 ANSWER 179 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439251-43-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopropanecarboxamide, N-[2-[4-(3-chlorobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-5-[(hexahydro-1H-1,4-diazepin-1-y1)carbonyl]phenyl]-(CA INDEX NAME)

MF C28 H34 C1 N5 O3

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 180 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439249-58-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Cyclopentanecarboxamide, N-[2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]-5-(1-piperazinylcarbonyl)phenyl]- (CA INDEX NAME)

MF C30 H36 F3 N5 O3

SR Chemical Library
Supplier: Ambinter

L18 ANSWER 181 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439249-01-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C32 H38 N6 O3

SR Chemical Library

Supplier: Ambinter

$$\begin{array}{c} \text{Me} \\ \text{C} \\ \text{N} \\ \text$$

L18 ANSWER 182 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-97-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C31 H35 C1 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 183 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-96-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]phenyl]-(CA INDEX NAME)

MF C32 H35 F3 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 184 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439248-93-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN 4-Pyridinecarboxamide, N-[5-[[(4-aminocyclohexyl)amino]carbonyl]-2-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]phenyl]- (CA INDEX NAME)

MF C32 H38 N6 O3

SR Chemical Library

Supplier: Ambinter

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L18 ANSWER 100 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN
RN 851164-41-5 REGISTRY
ED
    Entered STN: 26 May 2005
    Methanone, (4-cyclobutylhexahydro-1H-1, 4-diazepin-1-yl) [4-(3,5-
CN
     dimethyl-4-isoxazolyl)phenyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
    1H-1, 4-Diazepine, 1-cyclobutyl-4-[4-(3,5-dimethyl-4-
     isoxazolyl)benzoyl]hexahydro- (9CI)
     C21 H27 N3 O2
MF
CI
     COM
SR
     CA
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L18 ANSWER 125 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 851164-07-3 REGISTRY

ED Entered STN: 26 May 2005

CN [1,1'-Biphenyl]-4-carbonitrile, 4'-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-1,4-Diazepine, 1-[(4'-cyano[1,1'-biphenyl]-4-yl)carbonyl]-4-cyclobutylhexahydro- (9CI)

MF C23 H25 N3 O

CI COM

SR CA

L18 ANSWER 150 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439267-36-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[3-[(cyclobutylcarbonyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]-(CA INDEX NAME)

MF C34 H39 N5 O7

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 135 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439270-92-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[3-[(2-cyclopentyl-2-phenylacetyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]-4-methyl- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzenepropanoic acid, β -[[3-[(cyclopentylphenylacetyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]-4-methyl- (9CI)

MF C44 H50 N4 O7

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 130 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 443767-05-3 REGISTRY

ED Entered STN: 13 Aug 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propen-1-yl)amino]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propenyl)amino]-(9CI)

MF C36 H43 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 127 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 443767-30-4 REGISTRY

ED Entered STN: 13 Aug 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propen-1-yl)amino]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propenyl)amino]-(9CI)

MF C35 H41 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 126 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 749866-38-4 REGISTRY

ED Entered STN: 23 Sep 2004

CN 2-Naphthalenesulfonamide, N-[3-[[4-(cyclohexylmethyl)hexahydro-1H-1,4-diazepin-1-yl]carbonyl]phenyl]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-1,4-Diazepine, 1-(cyclohexylmethyl)hexahydro-4-[3-[(2-naphthalenylsulfonyl)amino]benzoyl]- (9CI)

MF C29 H35 N3 O3 S

CI COM

SR CA

SR

L18 ANSWER 128 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 443767-24-6 REGISTRY

ED Entered STN: 13 Aug 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-phenpropen-1-yl)amino] - (CA INDEX NAME)

OTHER CA INDEX NAMES:

Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-phenpropenyl)amino]- (9CI)

MF C35 H38 F3 N5 O3

Chemical Library

Supplier: Ambinter

L18 ANSWER 129 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 443767-06-4 REGISTRY

ED Entered STN: 13 Aug 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propen-1-yl)amino]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propenyl)amino]-(9CI)

MF C35 H41 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 131 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 443767-04-2 REGISTRY

ED Entered STN: 13 Aug 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propen-1-yl)amino]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propenyl)amino]-(9CI)

MF C35 H38 N6 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 132 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 443767-02-0 REGISTRY

ED Entered STN: 13 Aug 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(1-oxo-3-phenyl-2-propen-1-yl)amino]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzamide, N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(1-oxo-3-phenyl-2-propenyl)amino]- (9CI)

MF C34 H39 N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 133 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 443767-01-9 REGISTRY

ED Entered STN: 13 Aug 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-fluorobenzoyl)hexahydro-1H1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propen-1-yl)amino]- (CA
INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propenyl)amino]- (9CI)

MF C34 H38 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 134 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 443766-99-2 REGISTRY

ED Entered STN: 13 Aug 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propen-1-yl)amino]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(1-oxo-3-phenyl-2-propenyl)amino]-(9CI)

MF C34 H38 F N5 O3

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 136 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439270-90-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(2-cyclopentyl-2-phenylacetyl)amino]benzoyl]amino]-4-methyl- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzenepropanoic acid, β -[[4-[4-(4-cyanobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-3-[(cyclopentylphenylacetyl)amino]benzoyl]amino]-4-methyl-(9CI)

MF C43 H45 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 137 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439270-86-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(2-cyclopentyl-2-phenylacetyl)amino]benzoyl]amino]-4-methyl-(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzenepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(cyclopentylphenylacetyl)amino]benzoyl]amino]-4-methyl- (9CI)

MF C42 H46 N4 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 138 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439270-26-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[3-[(2-cyclopentyl-2-phenylacetyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 3-Pyridinepropanoic acid, β -[[3-[(cyclopentylphenylacetyl)amino]- 4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]- (9CI)

MF C42 H47 N5 O7

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 139 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439270-24-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(2-cyclopentyl-2-phenylacetyl)amino]benzoyl]amino]-(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 3-Pyridinepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(cyclopentylphenylacetyl)amino]benzoyl]amino]-(9CI)

MF C41 H42 N6 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 140 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439270-20-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(2-cyclopentyl-2-phenylacetyl)amino]benzoyl]amino]-(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 3-Pyridinepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(cyclopentylphenylacetyl)amino]benzoyl]amino]- (9CI)

MF C40 H43 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 141 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439269-70-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN 2-Thiophenepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(cyclohexylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C34 H37 N5 O5 S

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 142 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439269-69-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN 2-Thiophenepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(cyclohexylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C33 H38 N4 O5 S

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 143 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439269-60-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN 2-Thiophenepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(cyclobutylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C32 H33 N5 O5 S

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 144 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439269-59-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN 2-Thiophenepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(cyclobutylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C31 H34 N4 O5 S

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 145 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439269-30-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN 2-Thiophenepropanoic acid, β -[[4-[4-(4-cyanobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-3-[(cyclopropylcarbony1)amino]benzoy1]amino]- (CA INDEX NAME)

MF C31 H31 N5 O5 S

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 146 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439269-29-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN 2-Thiophenepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(cyclopropylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C30 H32 N4 O5 S

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 147 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439267-49-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[3-[(cyclohexylcarbonyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]-(CA INDEX NAME)

MF C36 H43 N5 O7

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 148 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439267-48-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[4-[4-(4-cyanobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-3-[(cyclohexylcarbony1)amino]benzoy1]amino]- (CA INDEX NAME)

MF C35 H38 N6 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 149 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439267-46-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(cyclohexylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C34 H39 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 151 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439267-35-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(cyclobutylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C33 H34 N6 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 152 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439267-33-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(cyclobutylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C32 H35 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 153 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439266-53-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[3-[(cyclopropylcarbonyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]-(CA INDEX NAME)

MF C33 H37 N5 O7

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 154 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439266-52-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridinepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(cyclopropylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C32 H32 N6 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 155 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439266-50-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN 3-Pyridine propanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-[(cyclopropylcarbonyl)amino]benzoyl]amino]- (CA INDEX NAME)

MF C31 H33 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 156 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439263-76-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[3-[(cyclohexylcarbonyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]-4-methyl- (CA INDEX NAME)

MF C38 H46 N4 O7

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 157 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439263-75-9 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(cyclohexylcarbonyl)amino]benzoyl]amino]-4-methyl-(CA INDEX NAME)

MF C37 H41 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 158 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439263-73-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-y1)-3-[(cyclohexylcarbonyl)amino]benzoyl]amino]-4-methyl- (CA INDEX NAME)

MF C36 H42 N4 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 159 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439263-65-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[3-[(cyclobutylcarbonyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]-4-methyl- (CA INDEX NAME)

MF C36 H42 N4 O7

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 160 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439263-64-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, $\beta-[[4-[4-(4-cyanobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-3-[(cyclobutylcarbony1)amino]benzoy1]amino]-4-methyl-(CA INDEX NAME)$

MF C35 H37 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 161 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439263-62-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-y1)-3-[(cyclobutylcarbonyl)amino]benzoyl]amino]-4-methyl- (CA INDEX NAME)

MF C34 H38 N4 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 162 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439263-21-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[3-[(cyclopropylcarbonyl)amino]-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]benzoyl]amino]-4-methyl- (CA INDEX NAME)

MF C35 H40 N4 O7

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 163 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439263-20-4 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-[(cyclopropylcarbonyl)amino]benzoyl]amino]-4-methyl-(CA INDEX NAME)

MF C34 H35 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 164 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439263-19-1 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, β -[[4-(4-benzoylhexahydro-1H-1,4-diazepin-1-y1)-3-[(cyclopropylcarbonyl)amino]benzoyl]amino]-4-methyl- (CA INDEX NAME)

MF C33 H36 N4 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 165 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439259-17-3 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methylbenzoyl)-1H-1,4-diazepin-1-yl]-3-nitro- (CA INDEX NAME)

MF C26 H33 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 166 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439259-11-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-chlorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-nitro- (CA INDEX NAME)

MF C25 H30 C1 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 167 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439259-10-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-[3-(trifluoromethyl)benzoyl]-1H-1,4-diazepin-1-yl]-3-nitro- (CA INDEX NAME)

MF C26 H30 F3 N5 O4

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 168 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439259-08-2 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[hexahydro-4-(3-methoxybenzoyl)-1H-1,4-diazepin-1-yl]-3-nitro- (CA INDEX NAME)

MF C26 H33 N5 O5

SR Chemical Library

Supplier: Ambinter

L18 ANSWER 169 OF 381 REGISTRY COPYRIGHT 2009 ACS on STN

RN 439259-06-0 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3,4-dimethoxybenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-nitro- (CA INDEX NAME)

MF C27 H35 N5 O6

SR Chemical Library

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ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-cyanobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-nitro- (CA INDEX NAME)

MF C26 H30 N6 O4

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RN 439259-02-6 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-(4-benzoylhexahydro-1H-1,4-diazepin-1-yl)-3-nitro- (CA INDEX NAME)

MF C25 H31 N5 O4

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RN 439259-01-5 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(3-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-nitro- (CA INDEX NAME)

MF C25 H30 F N5 O4

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RN 439258-99-8 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzamide, N-(4-aminocyclohexyl)-4-[4-(4-fluorobenzoyl)hexahydro-1H-1,4-diazepin-1-yl]-3-nitro- (CA INDEX NAME)

MF C25 H30 F N5 O4

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RN 439252-70-7 REGISTRY

ED Entered STN: 18 Jul 2002

CN Benzenepropanoic acid, $\beta-[[4-[4-(4-cyanobenzoy1)hexahydro-1H-1,4-diazepin-1-y1]-3-[(cyclohexylcarbonyl)amino]benzoy1]amino]-4-fluoro-(CA INDEX NAME)$

MF C36 H38 F N5 O5

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